

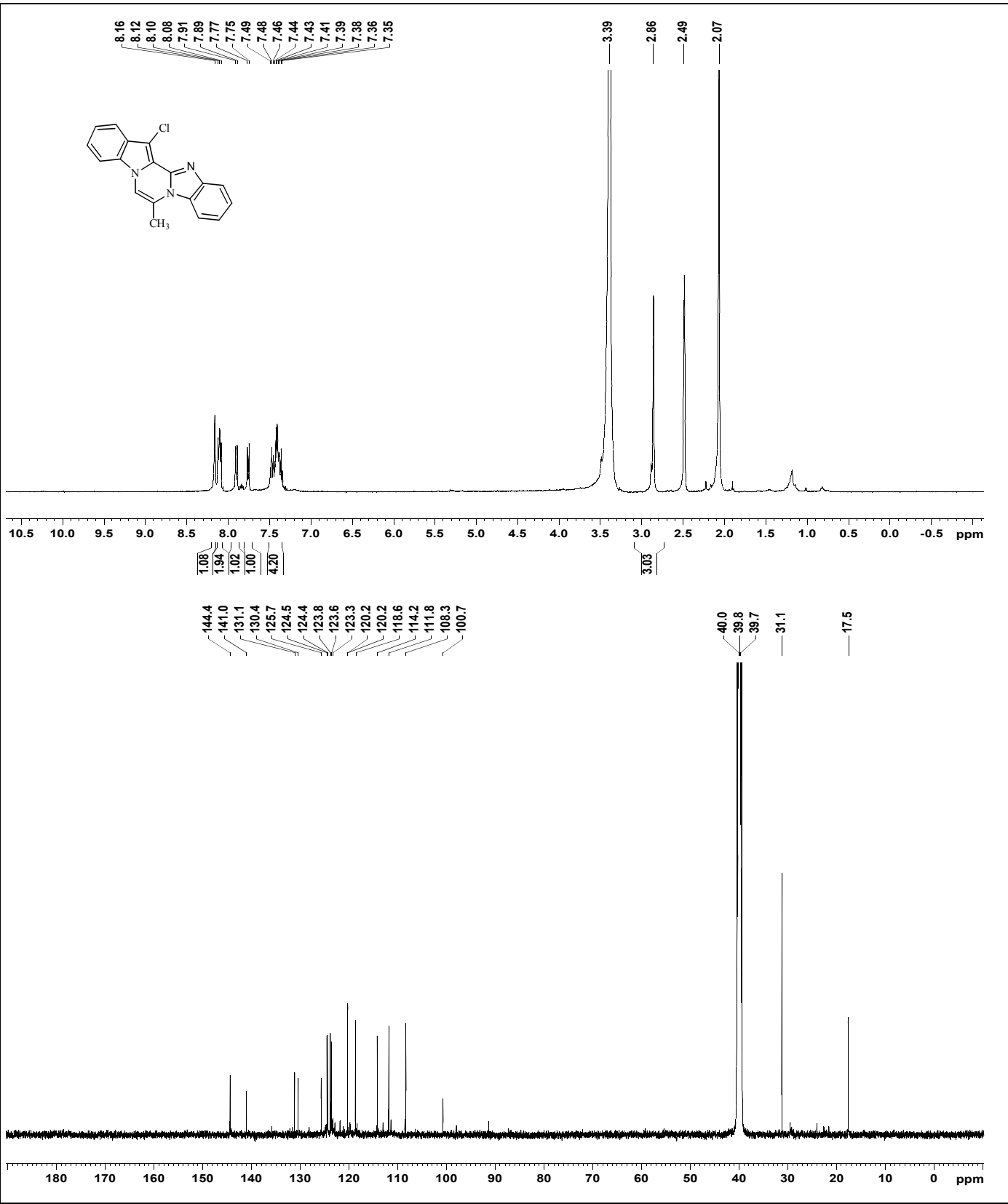
Supplementary Information

Copper Catalyzed Synthesis of Fused Benzimidazolopyrazine Derivatives via Tandem Benzimidazole formation/Annulation of δ - alkynylaldehyde

Subburethinam Ramesh, Suman Kr Ghosh and Rajagopal Nagarajan*

^1H and ^{13}C spectra of 3a-r, 5a-c, 7a-c

¹H and ¹³C Spectra of 3a

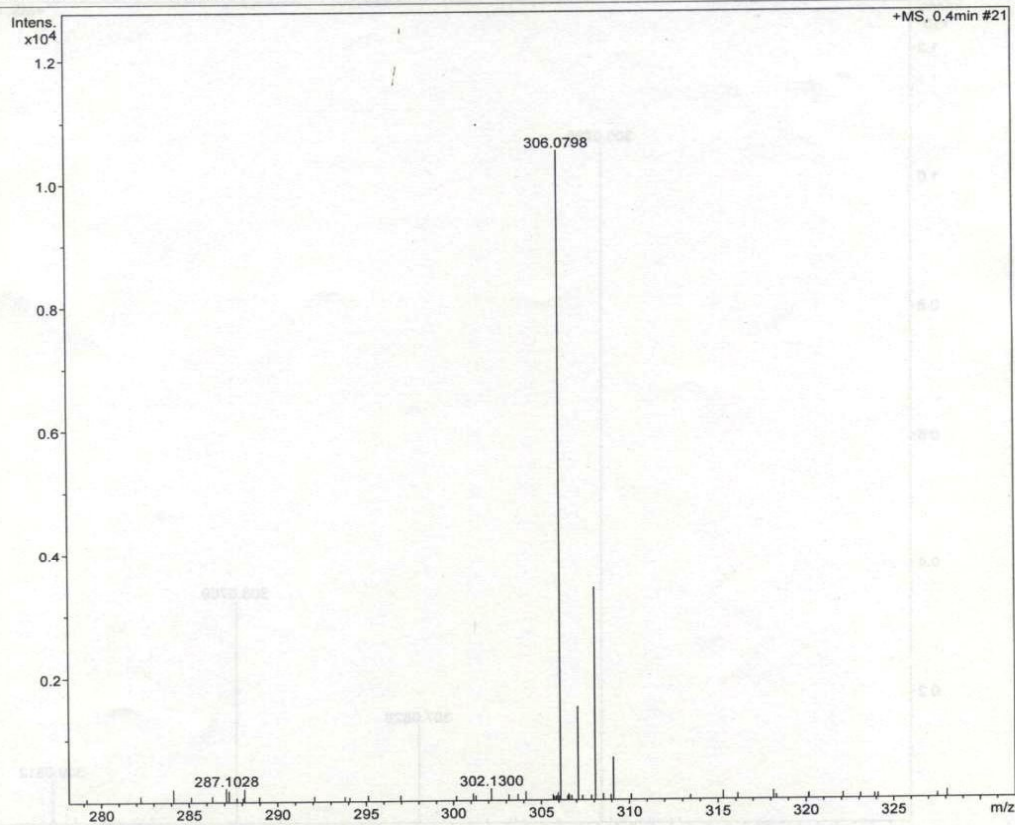


HRMS of 3a

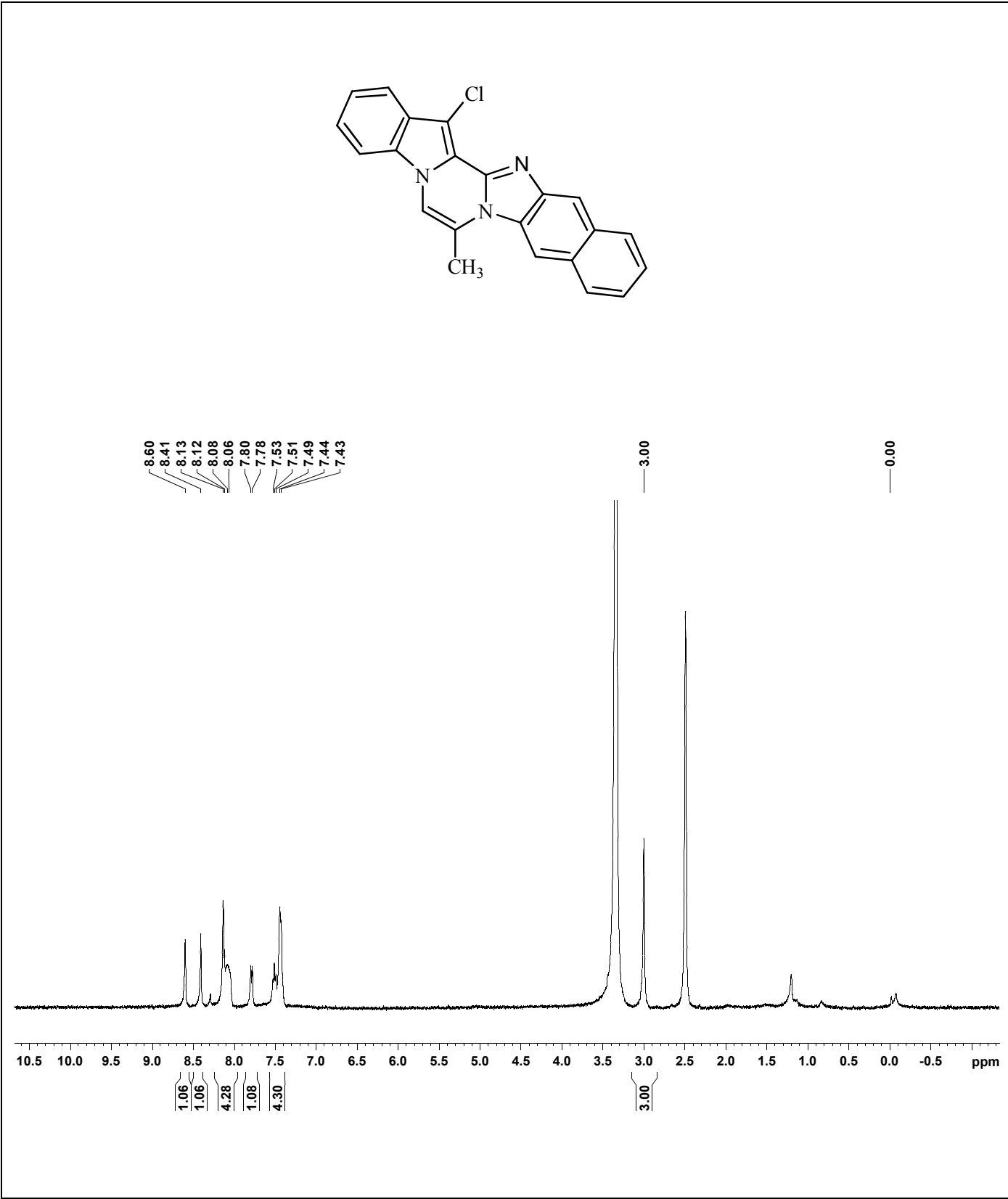
BRUKER MAXIS HRMS REPORT
SCHOOL OF CHEMISTRY

Analysis Info		Acquisition Date	10/5/2012 10:14:14 AM
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Method	tune_low.m	Instrument	maXis
Sample Name	SRM-500-DCM-MEOH		10138
Comment			

Acquisition Parameter		Ion Polarity	Positive	Set Nebulizer	4.4 psi
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Focus	Not active	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan Begin	50 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste
Scan End	1500 m/z				



¹H Spectrum of 3b



HRMS of 3b

BRUKER MAXIS HRMS REPORT SCHOOL OF CHEMISTRY

Analysis Info

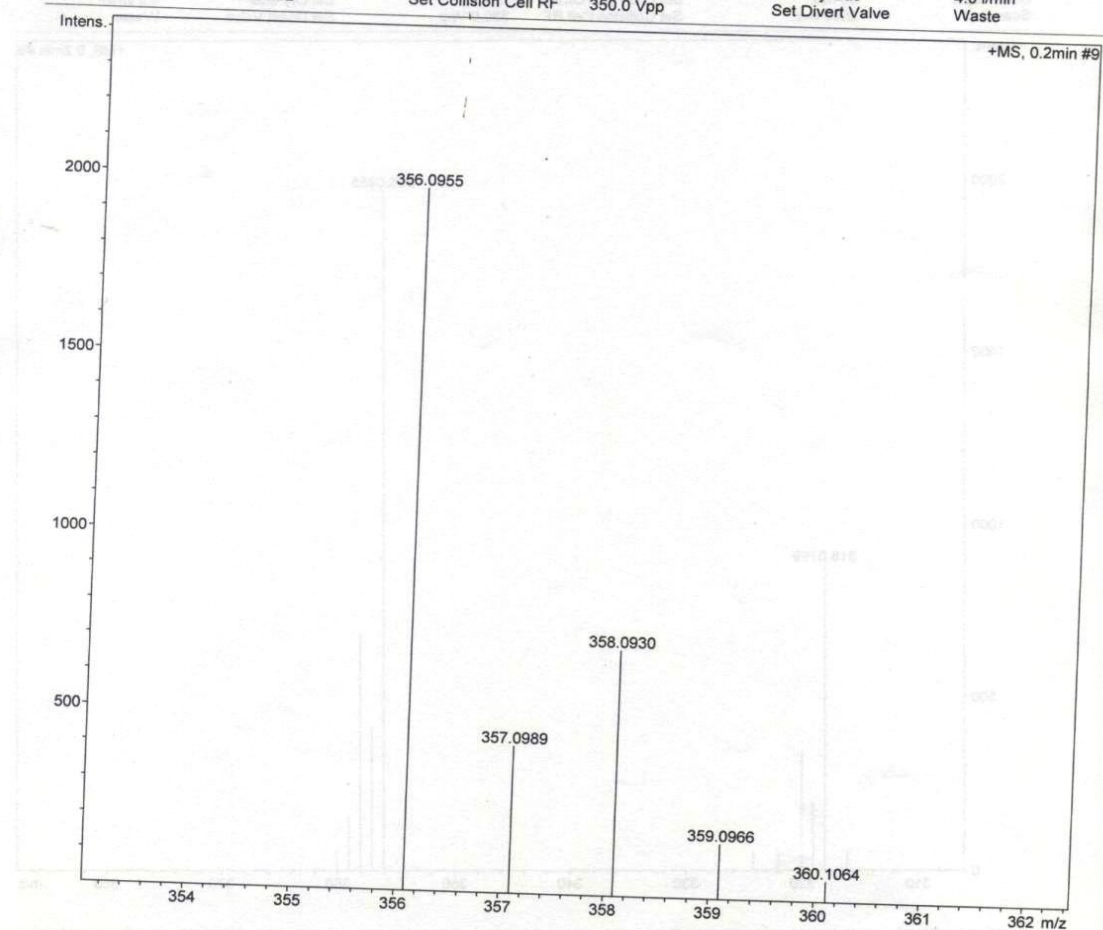
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Sample Name SRM-507DCM-MEOH
Comment

Acquisition Date 10/5/2012 10:47:10 AM

Operator UOH
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
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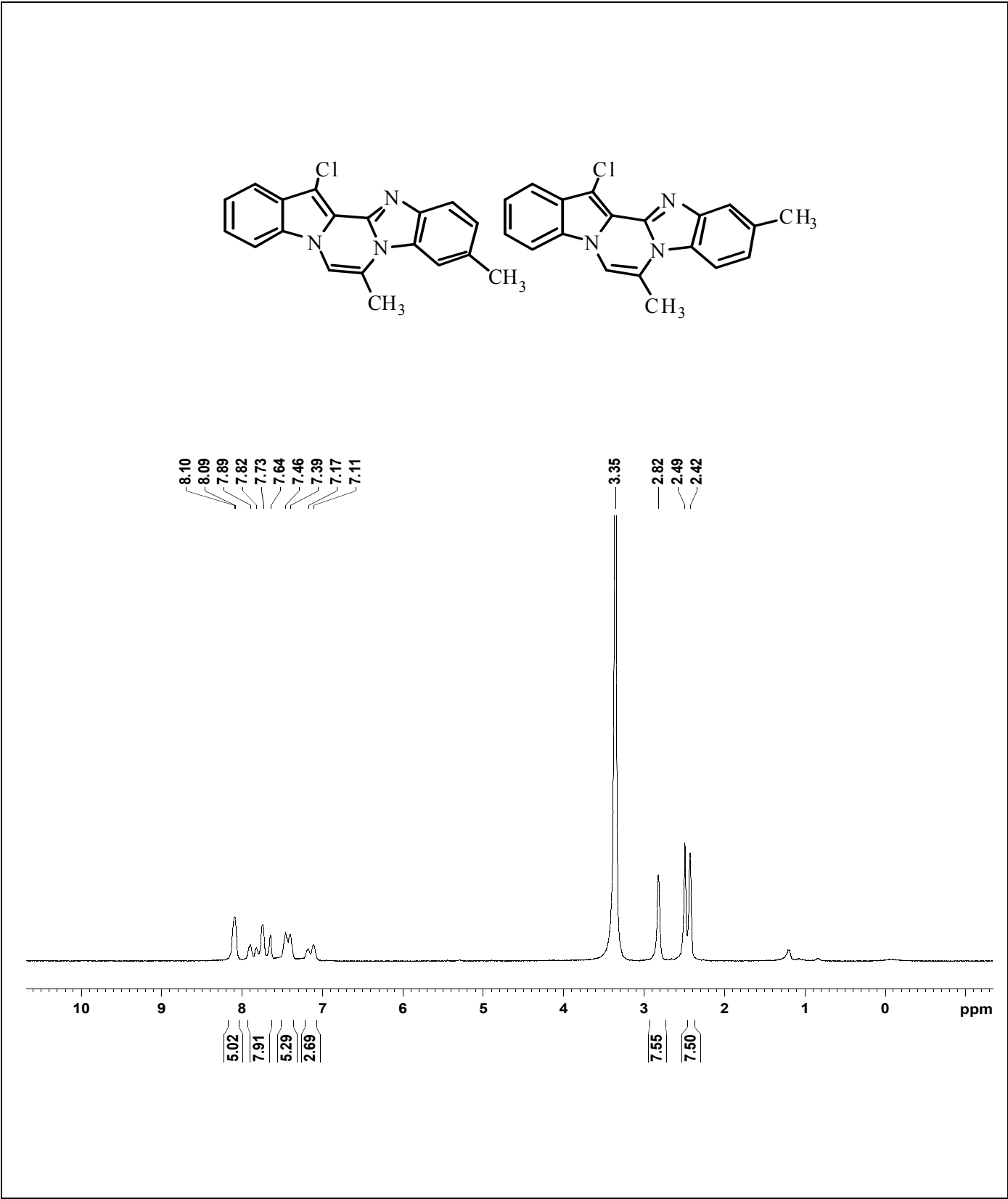


Bruker Compass DataAnalysis 4.0

printed: 10/5/2012 10:55:39 AM

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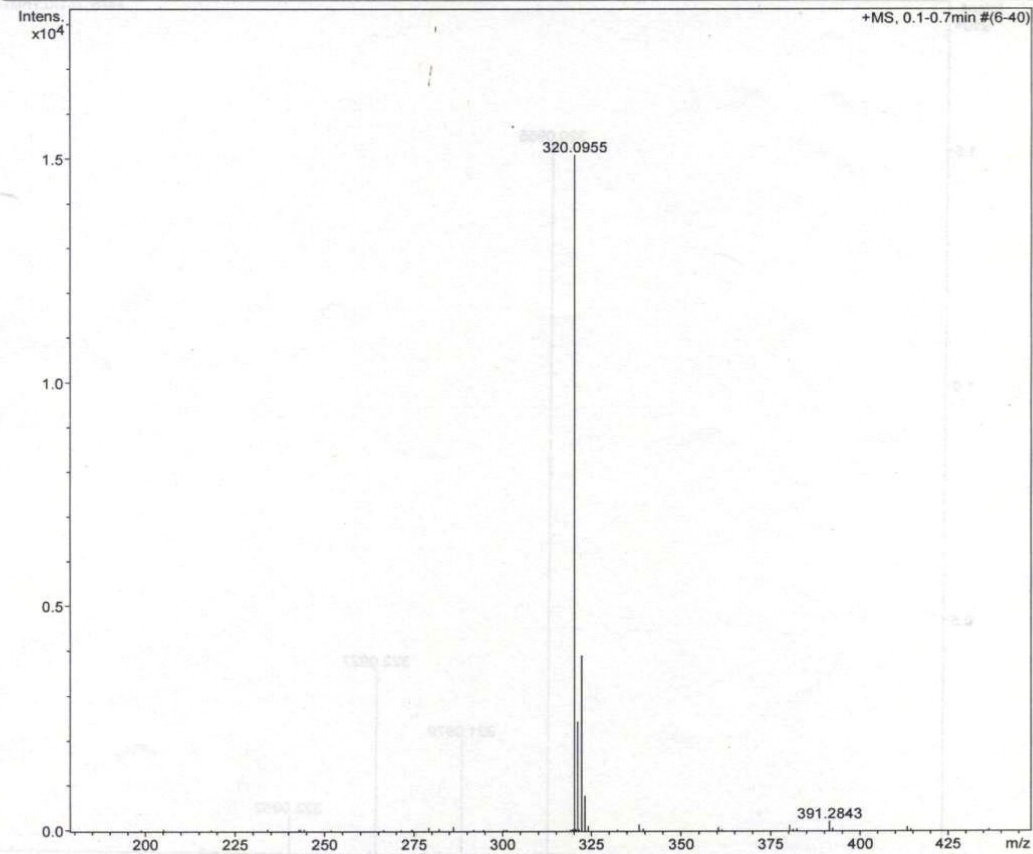
¹H Spectrum of 3c and 3c'



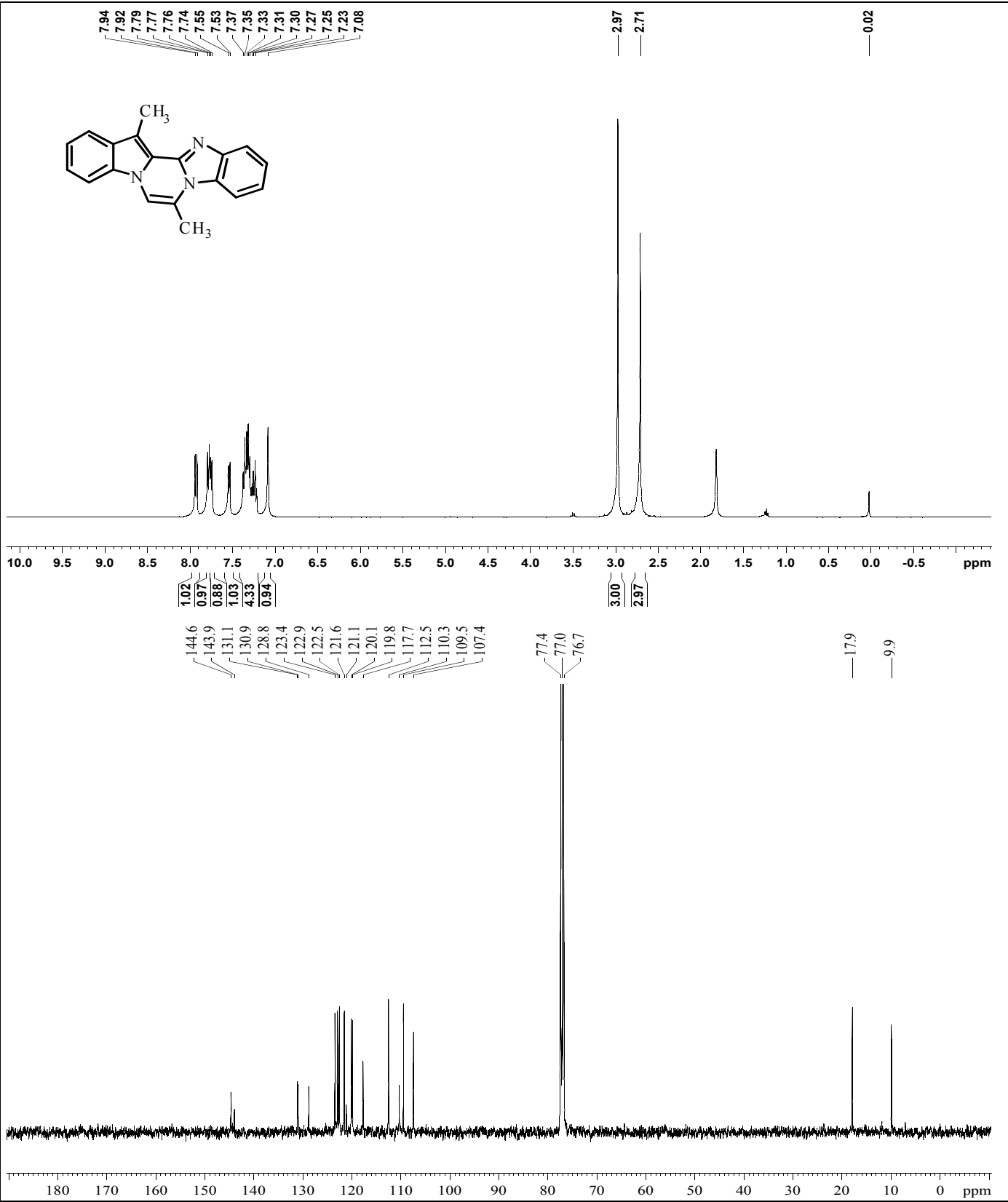
HRMS of 3c and 3c'

BRUKER MAXIS HRMS REPORT
SCHOOL OF CHEMISTRY

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Method	tune_low_Pos.m			Instrument	maXis	
Sample Name	SRM-508-DCM-MEOH				10138	
Comment						
Acquisition Parameter						
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min	
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste	



¹H and ¹³C Spectra of 3d



HRMS of 3d

BRUKER MAXIS HRMS REPORT SCHOOL OF CHEMISTRY

Analysis Info

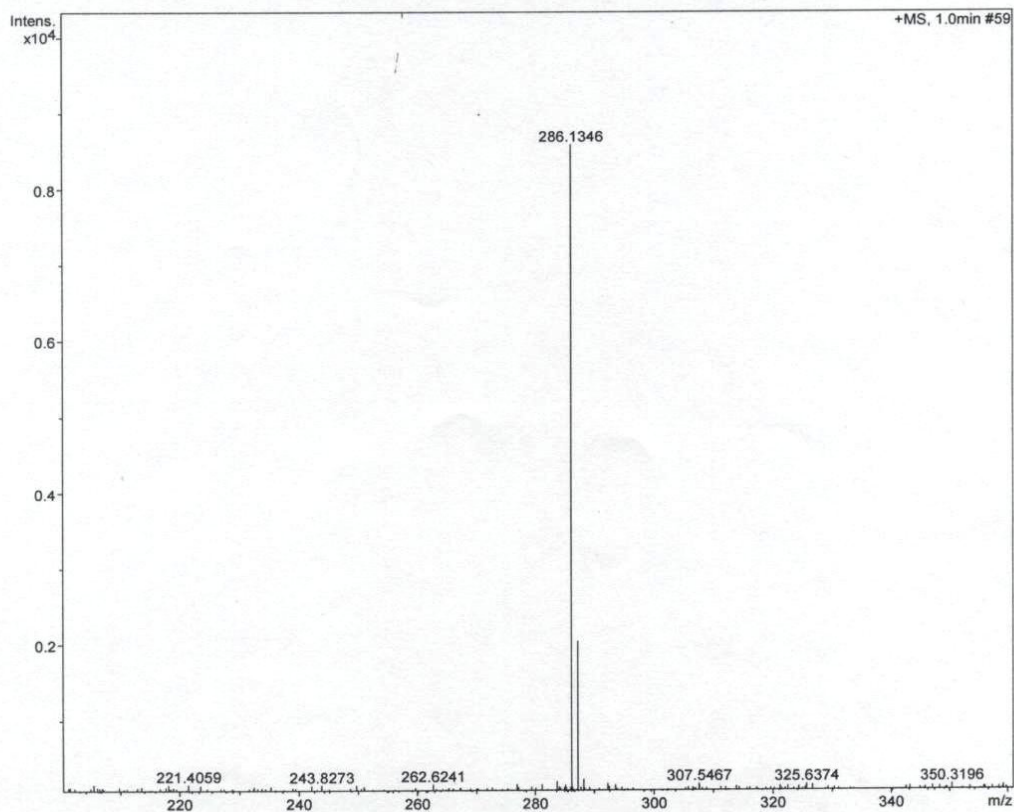
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Sample Name SRM-306-DCM-MEOH
Comment

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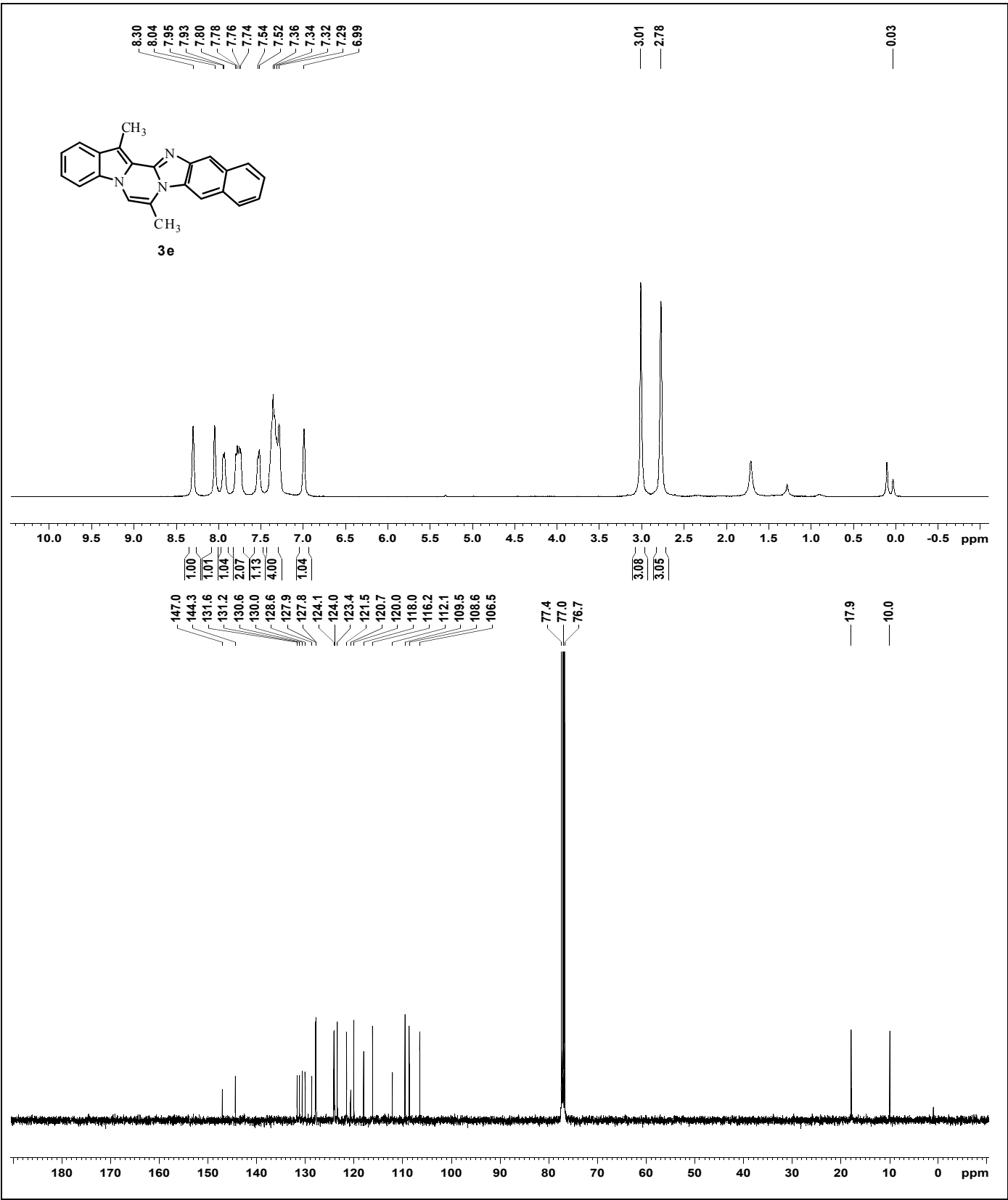
Operator UOH
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 3e



HRMS of 3e

BRUKER MAXIS HRMS REPORT SCHOOL OF CHEMISTRY

Analysis Info

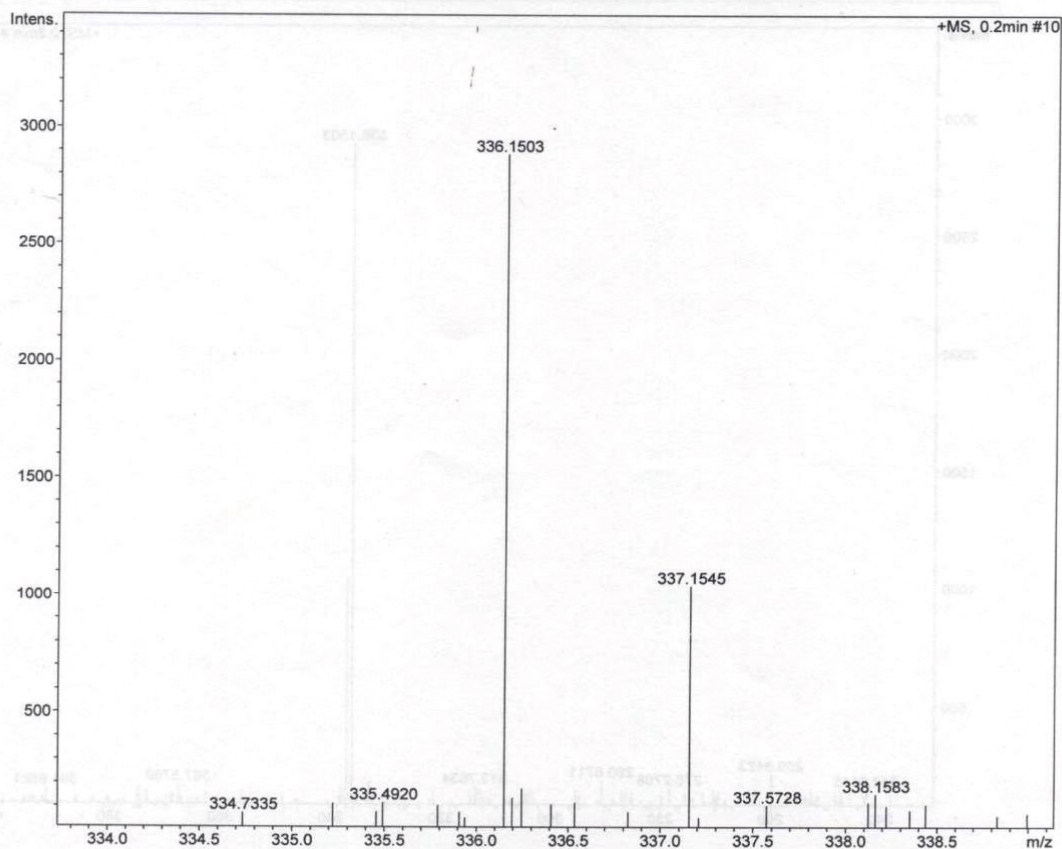
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Sample Name SRM-521-CM-MEOH
Comment

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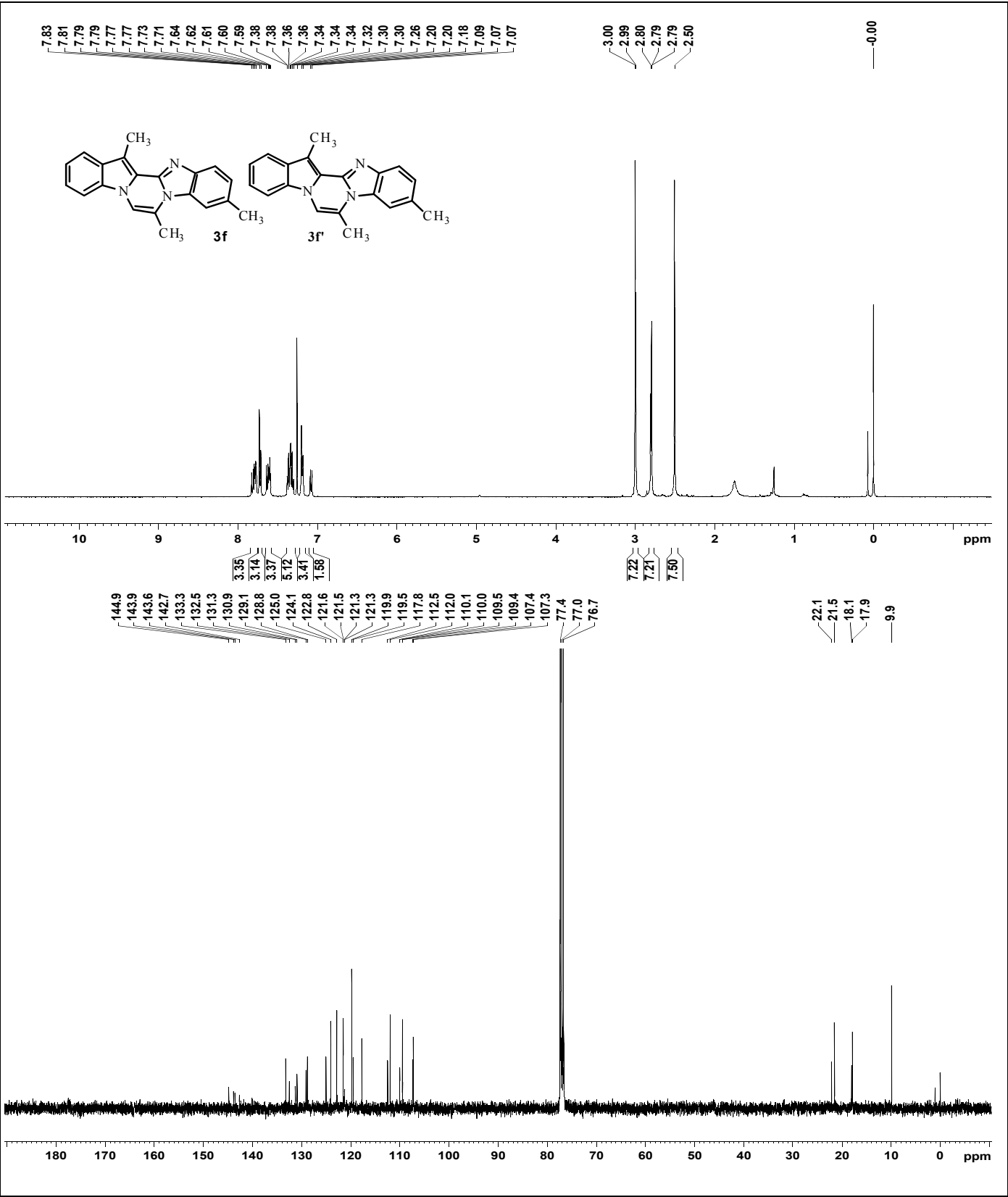
Operator UOH
Instrument maXis 10138

Acquisition Parameter

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Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 3f and 3f'



HRMS of 3f and 3ff

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Analysis Info

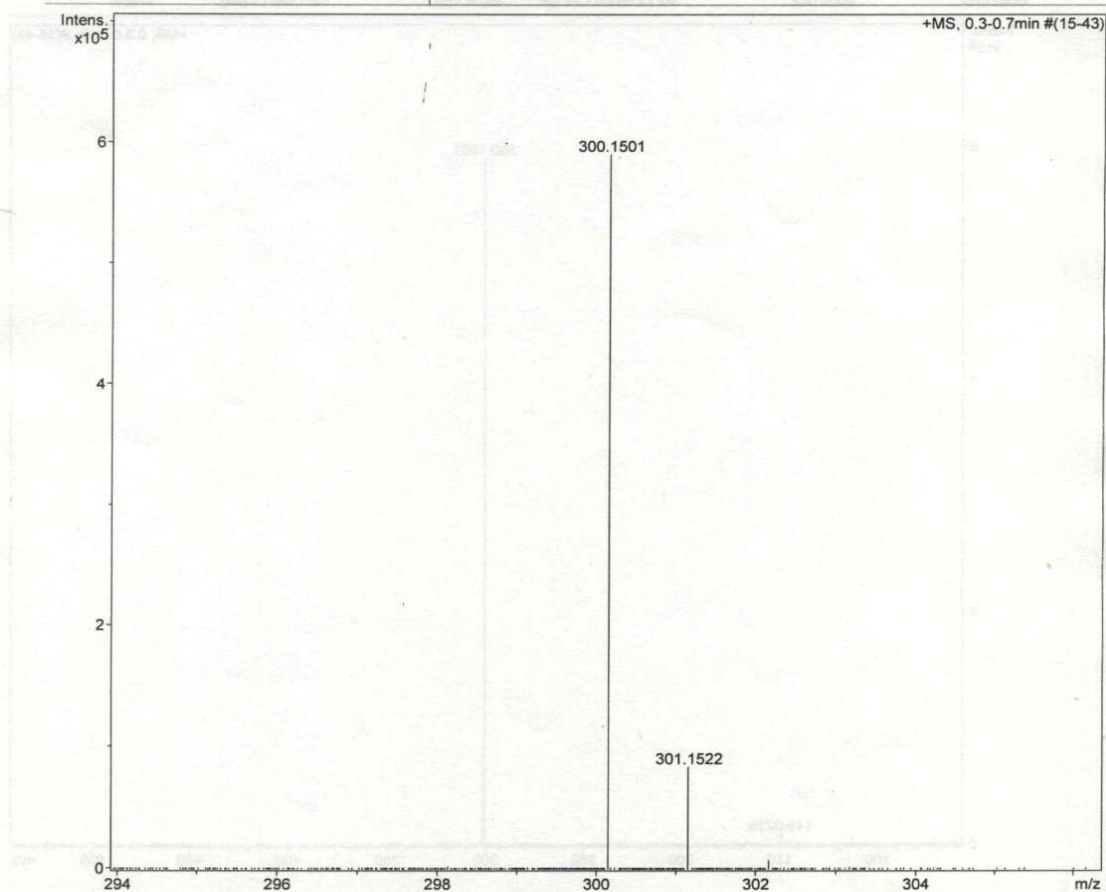
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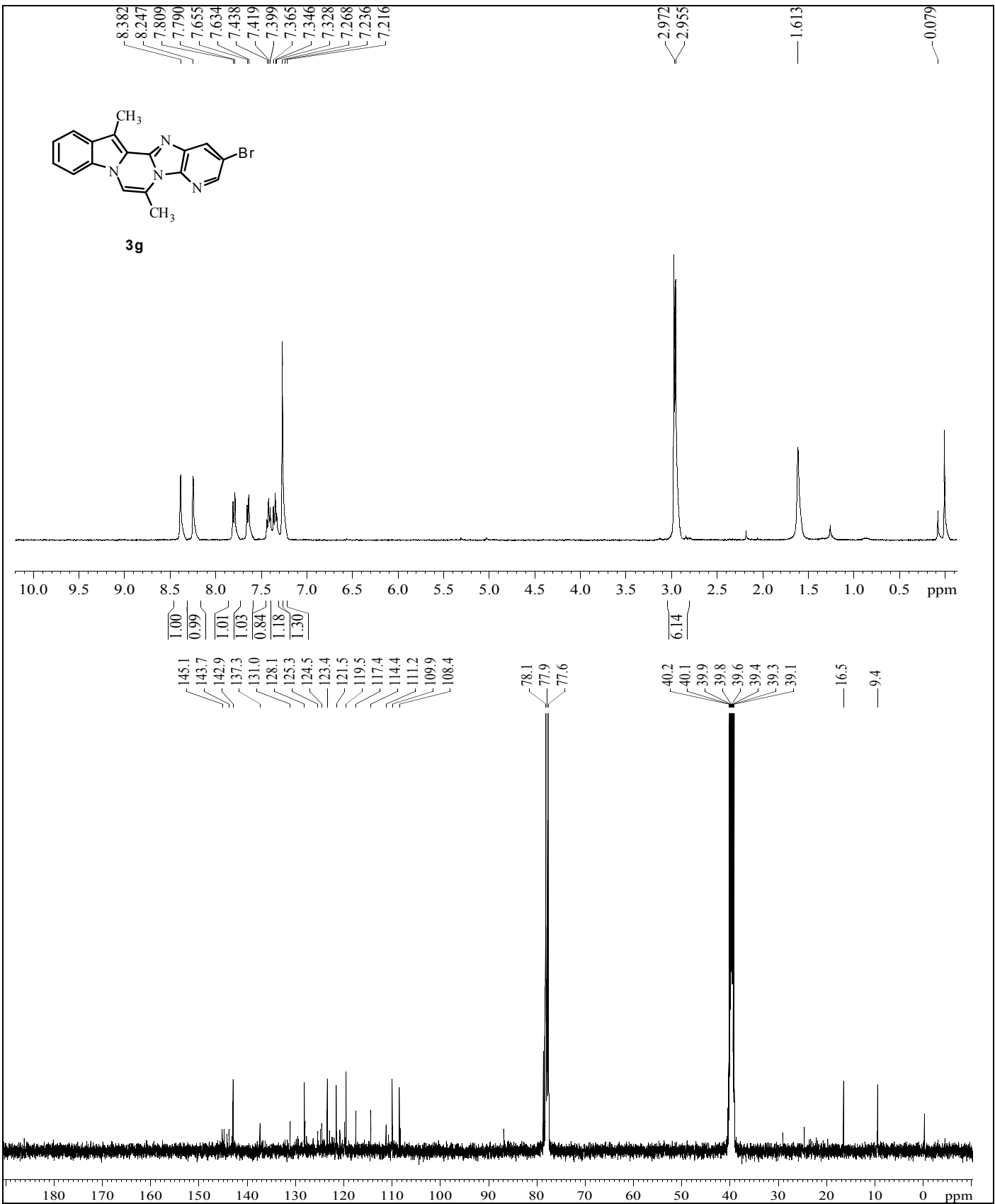
Operator UOH
Instrument maXis 10138

Acquisition Parameter

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Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 3g



HRMS of 3g

BRUKER MAXIS HRMS REPORT SCHOOL OF CHEMISTRY

Analysis Info

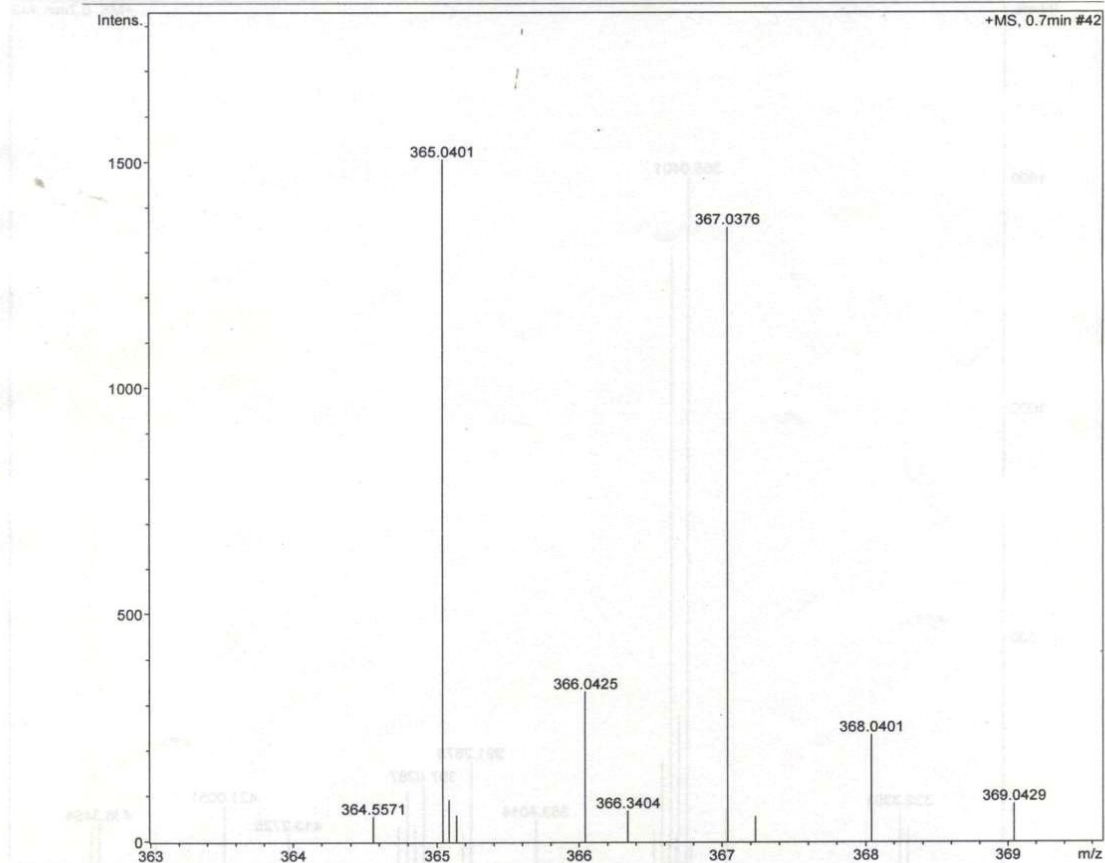
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Sample Name SRM-SKG-62-DCM-MEOH
Comment

Acquisition Date 10/5/2012 11:03:45 AM

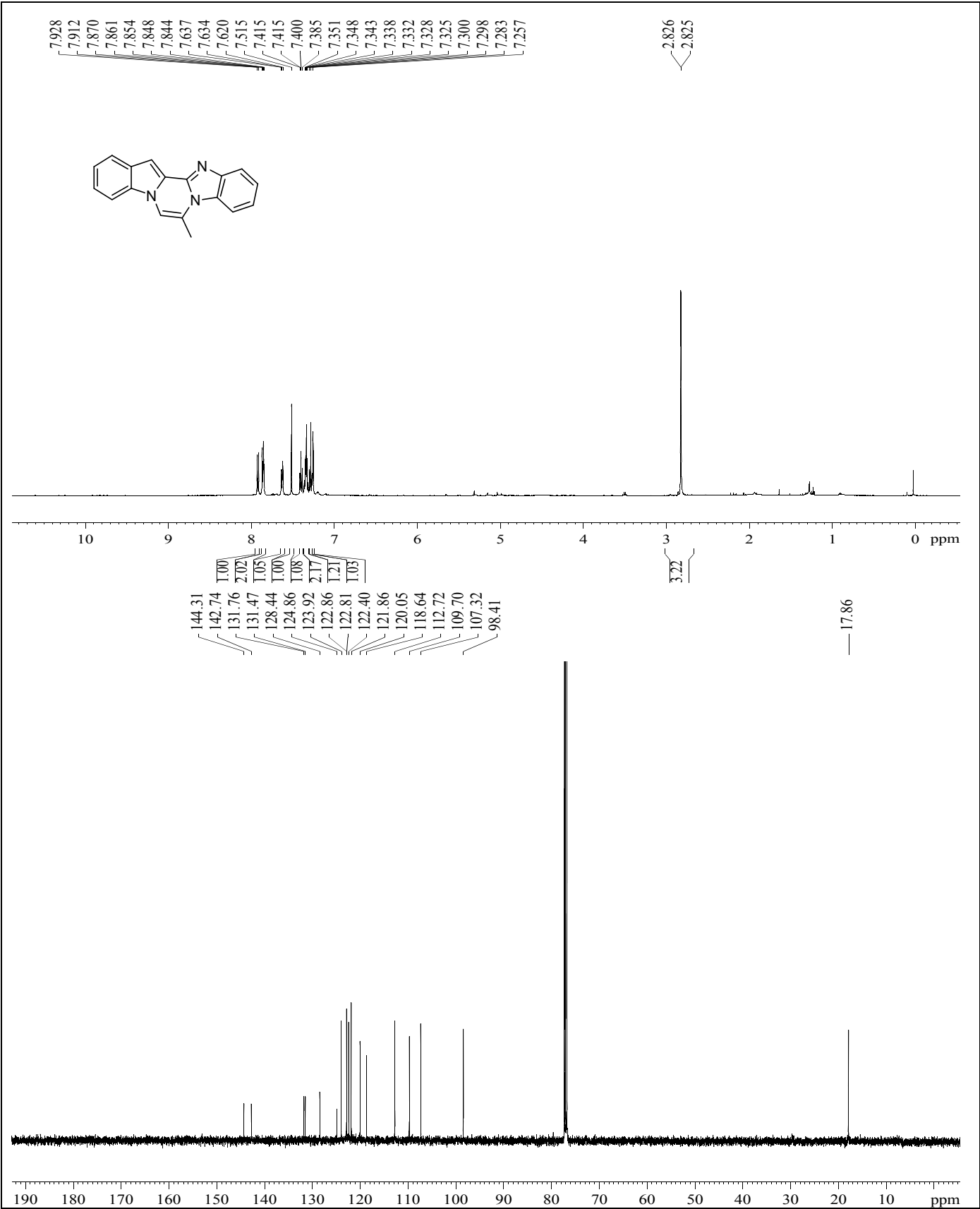
Operator UOH
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 3h



HRMS of 3h

BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

Analysis Name D:\Data\2013\Dr.NAGARAJAN\APR\SRM-639.d
Method tune_low.m
Sample Name SRM-639-DCM-MEOH
Comment

Acquisition Date 4/18/2013 3:43:34 PM

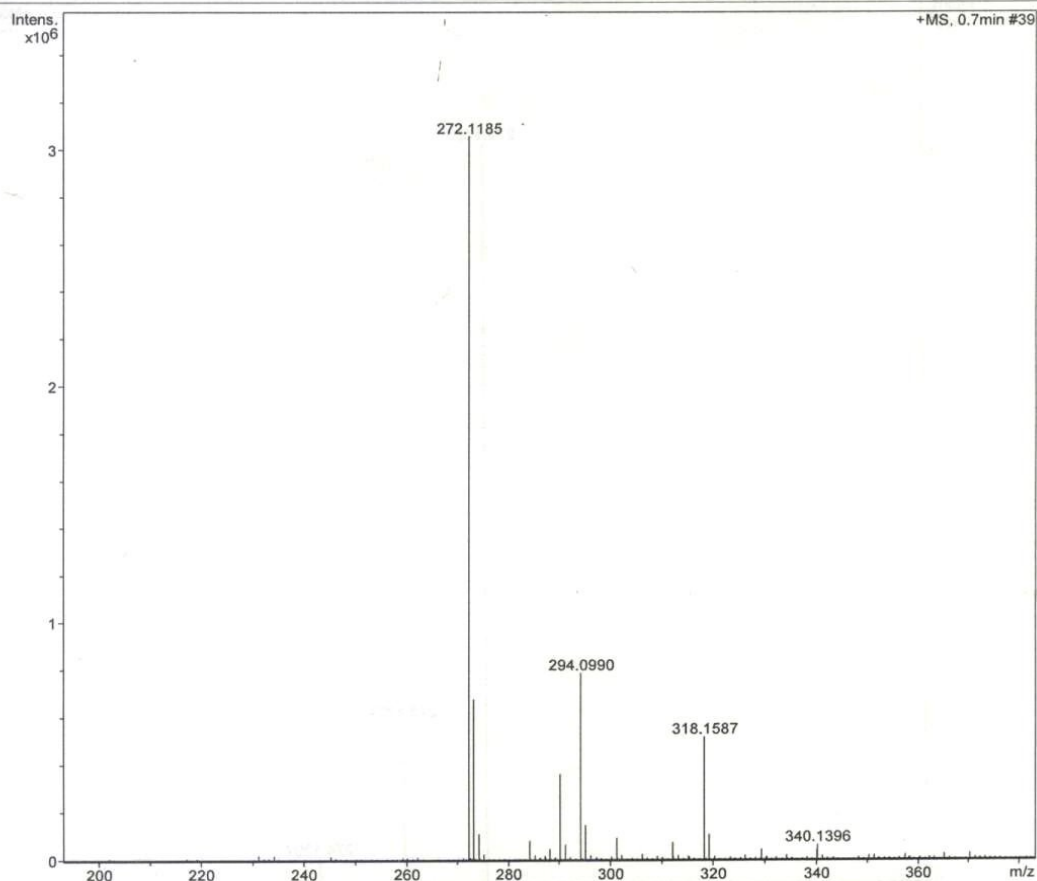
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

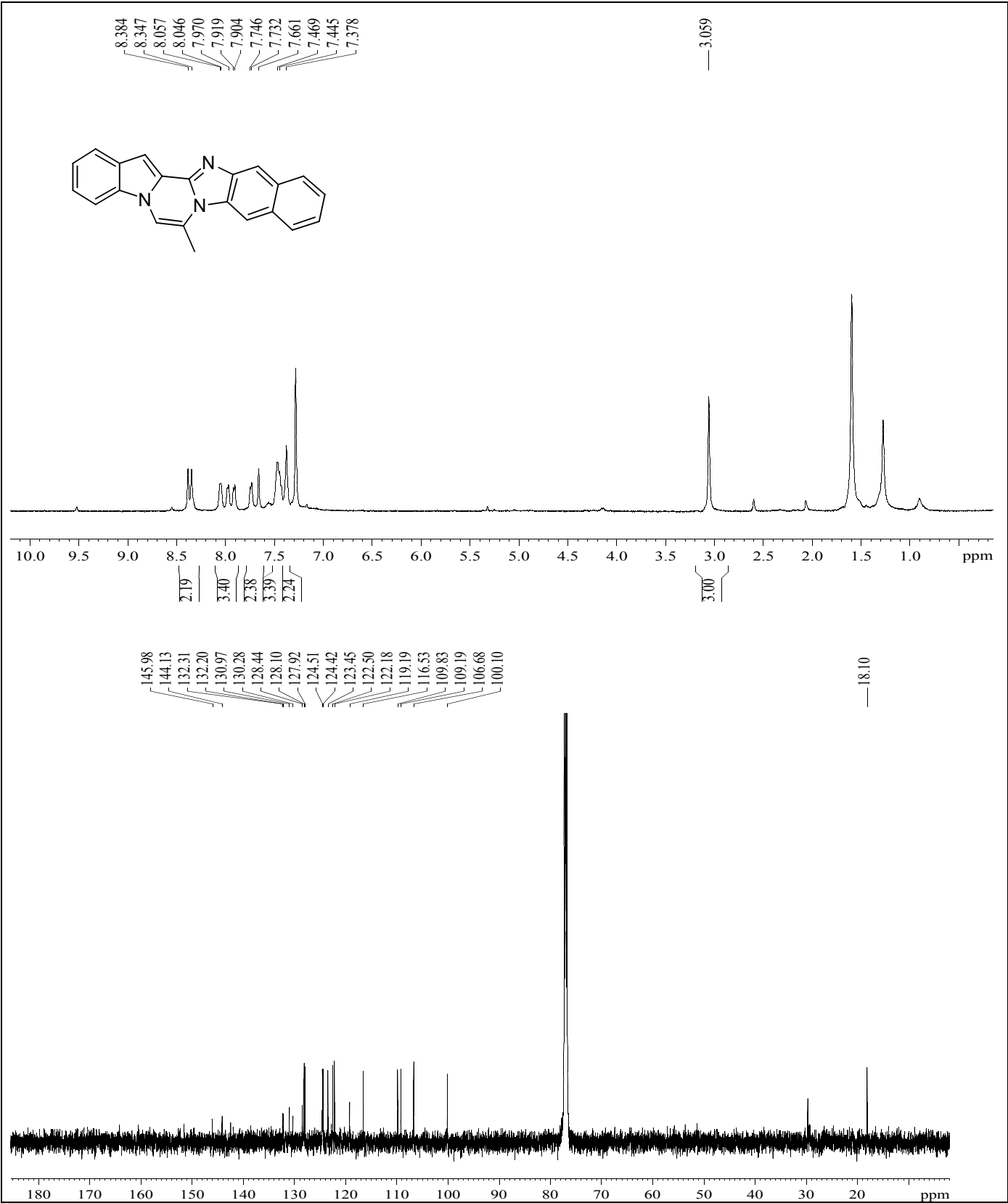
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Scan End 1800 m/z

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Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 4.4 psi
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste



¹H and ¹³C Spectra of 3i



HRMS of 3i

BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

Analysis Name D:\Data\2013\Dr.NAGARAJAN\APR\SRM-640.d
Method tune_low.m
Sample Name SRM-640-DCM-MEOH
Comment

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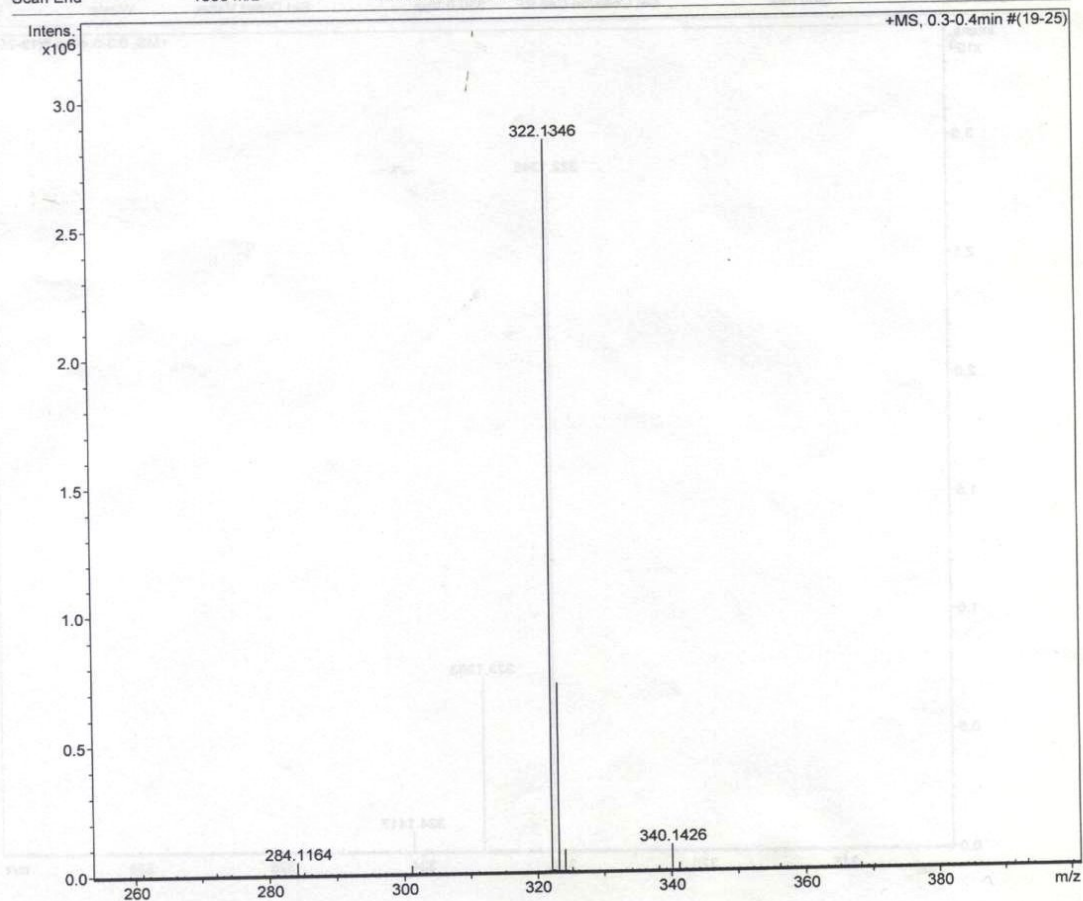
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

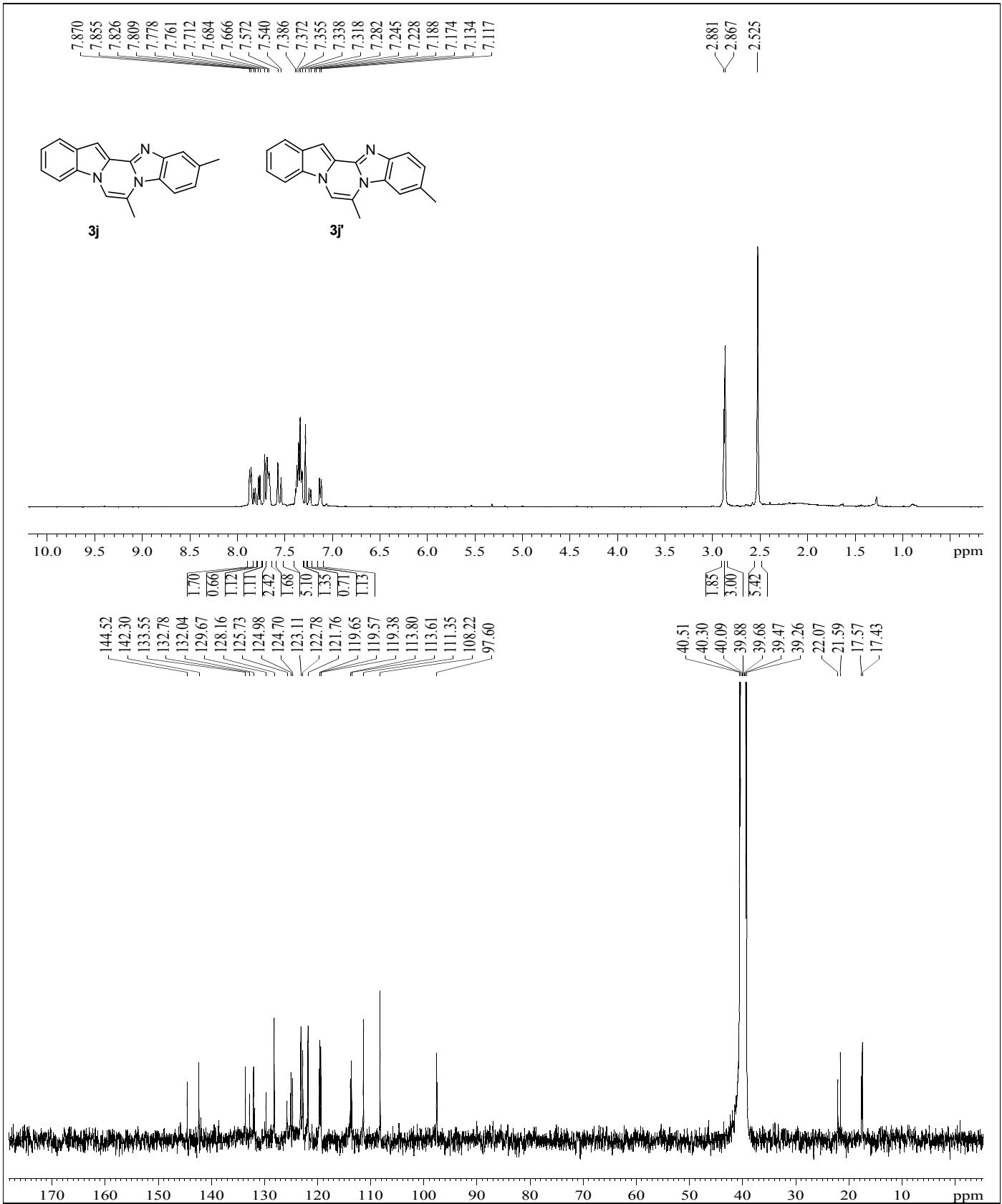
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Focus Not active
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Ion Polarity Positive
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Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 4.4 psi
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste



¹H and ¹³C Spectra of 3j and 3j'



HRMS of 3j and 3j'

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Analysis Info

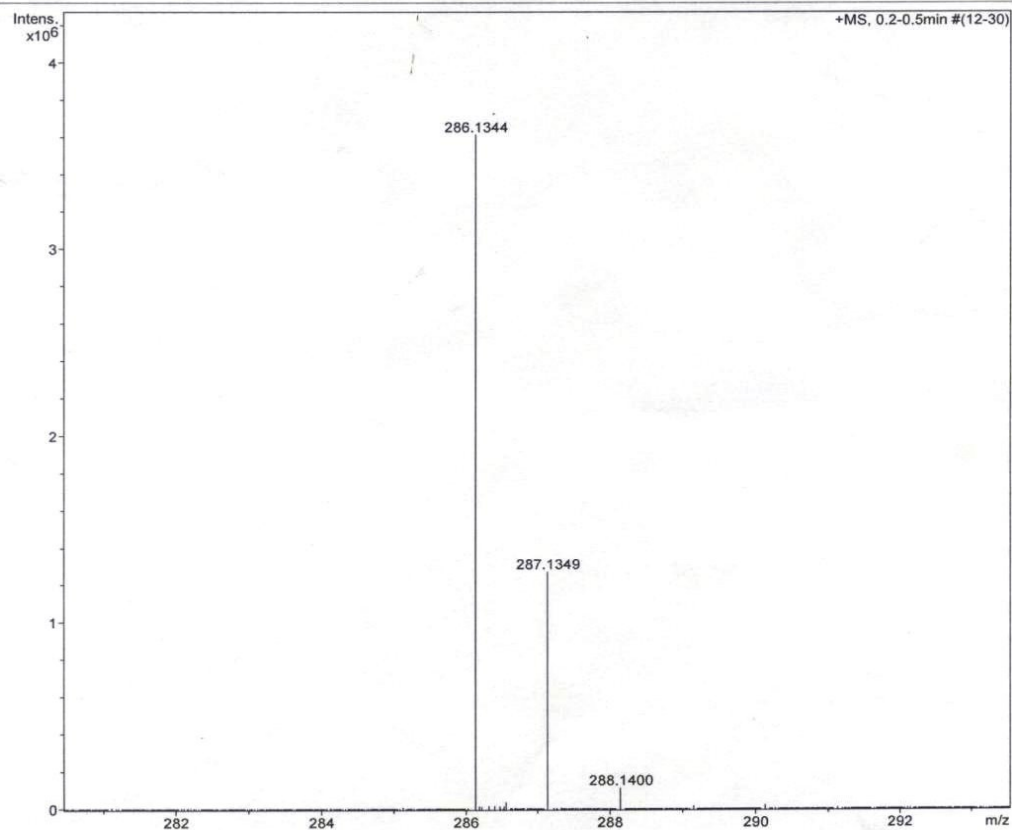
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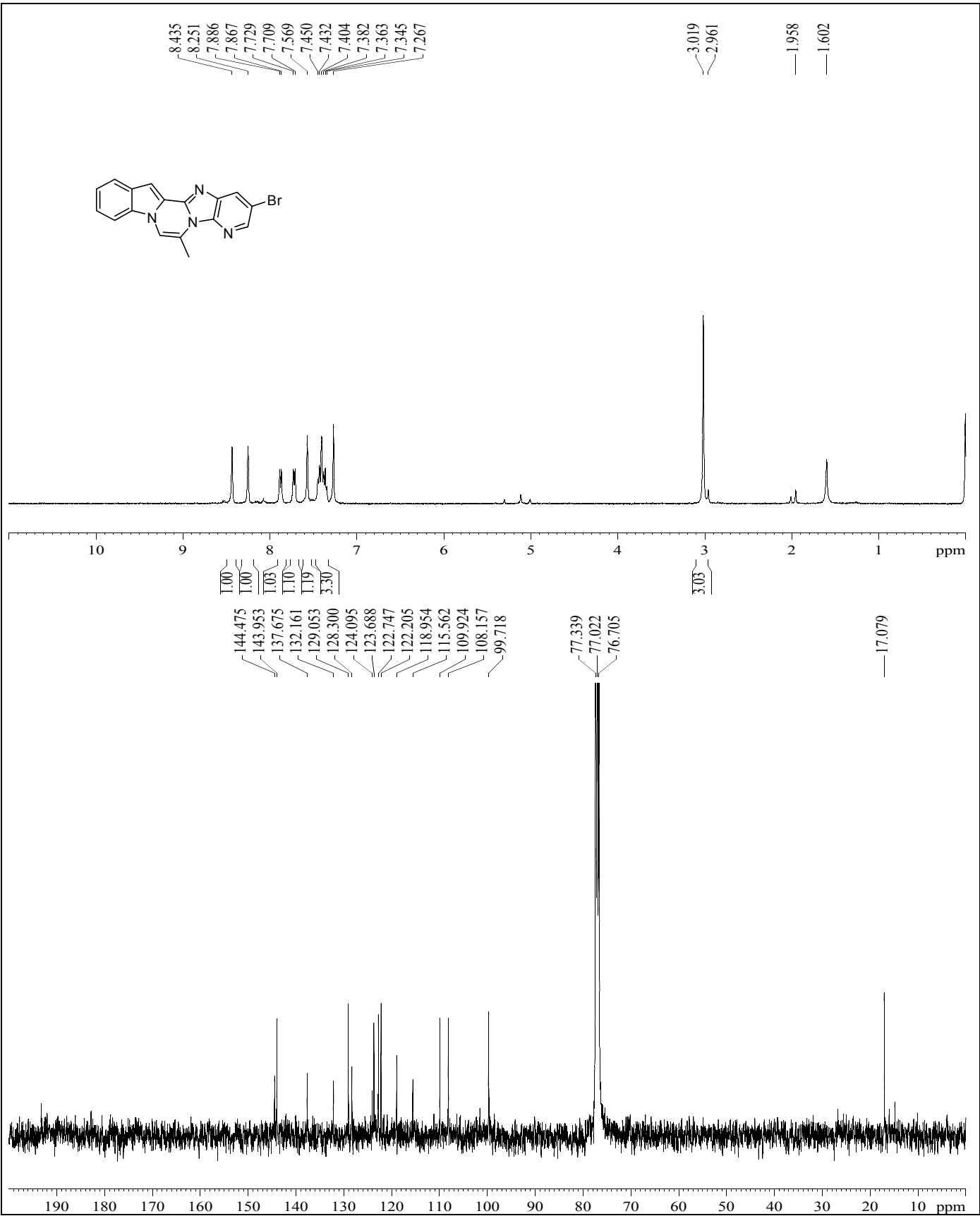
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
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Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 3k



HRMS of 3k

BRUKER MAXIS HRMS REPORT

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Analysis Info

Analysis Name D:\Data\2013\Dr.NAGARAJAN\APR\SRM-641R.d
Method tune_low.m
Sample Name SRM-641R--DCM-MEOH
Comment

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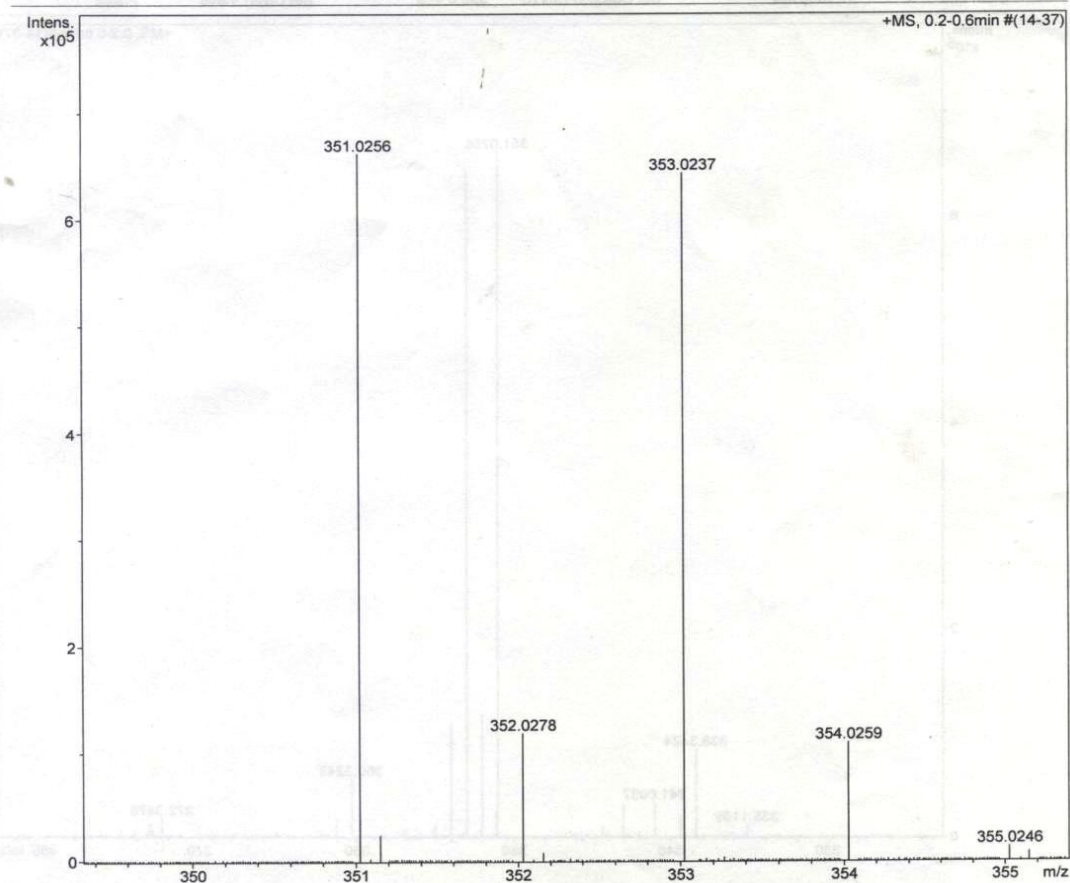
Operator Ramu Sridhar
Instrument maXis 10138

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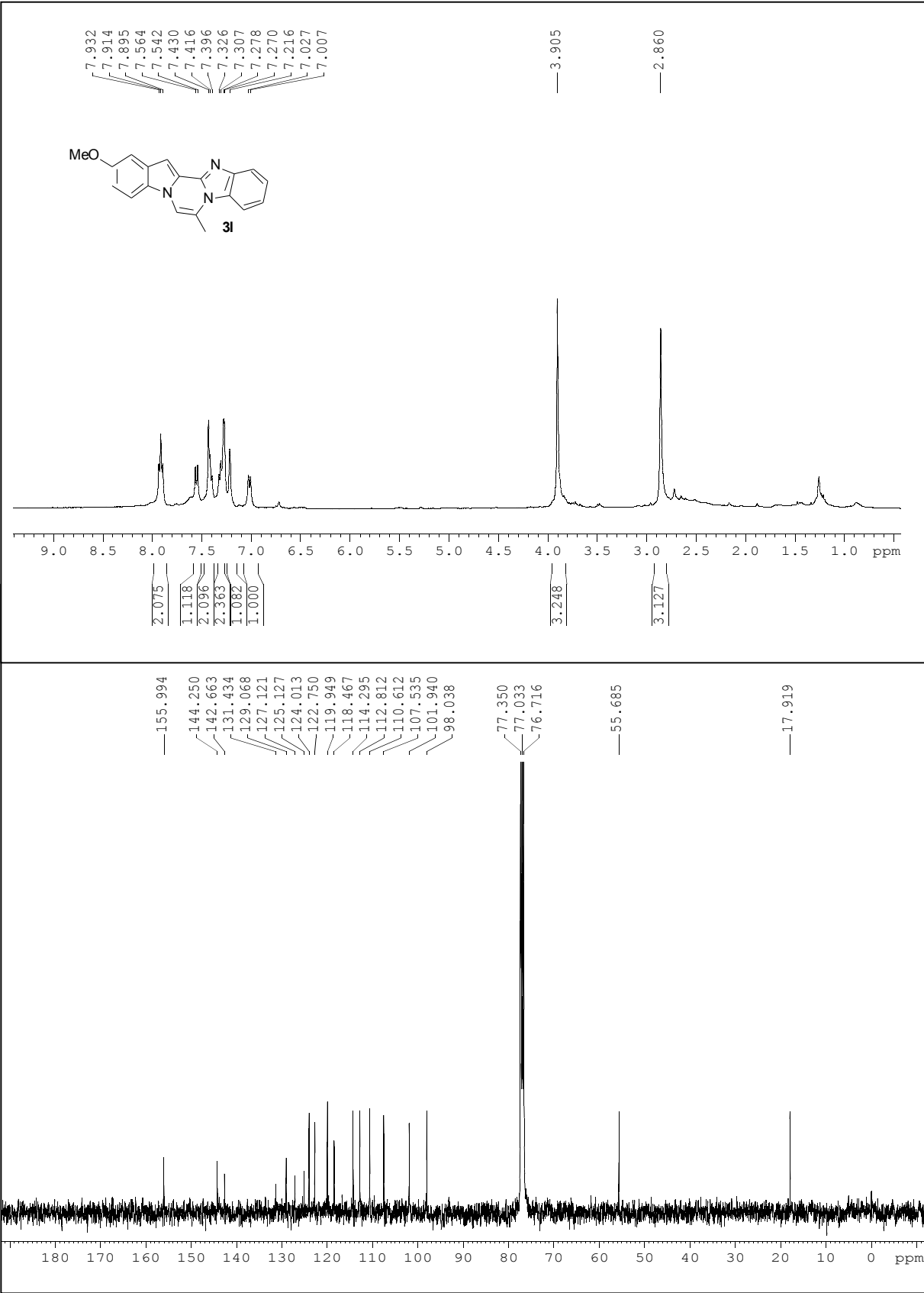
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Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 4.4 psi
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste



¹H and ¹³C spectra of compounds 3I



HRMS of 3I

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Analysis Info

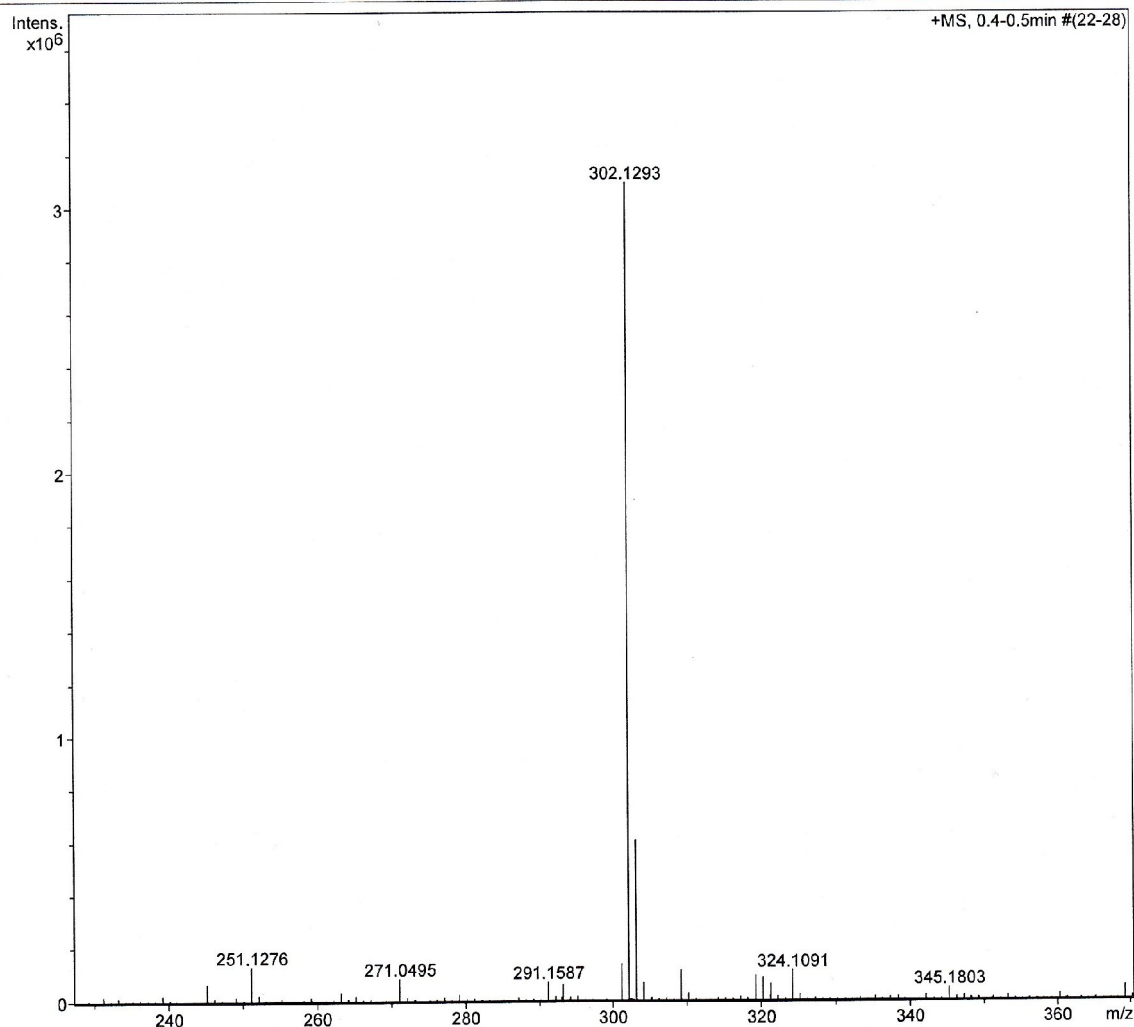
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Comment

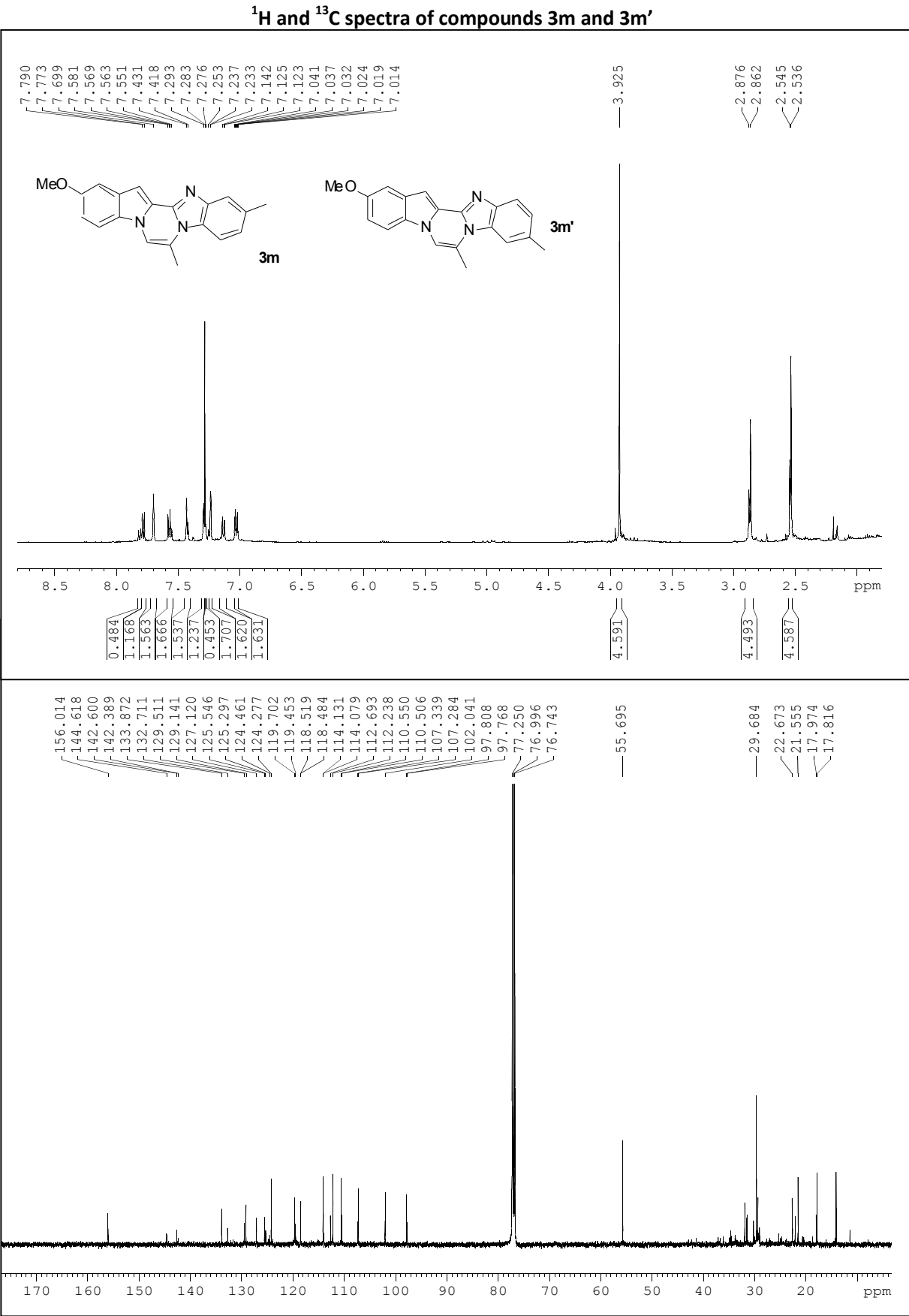
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Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





HRMS of 3m and 3m'

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Analysis Info

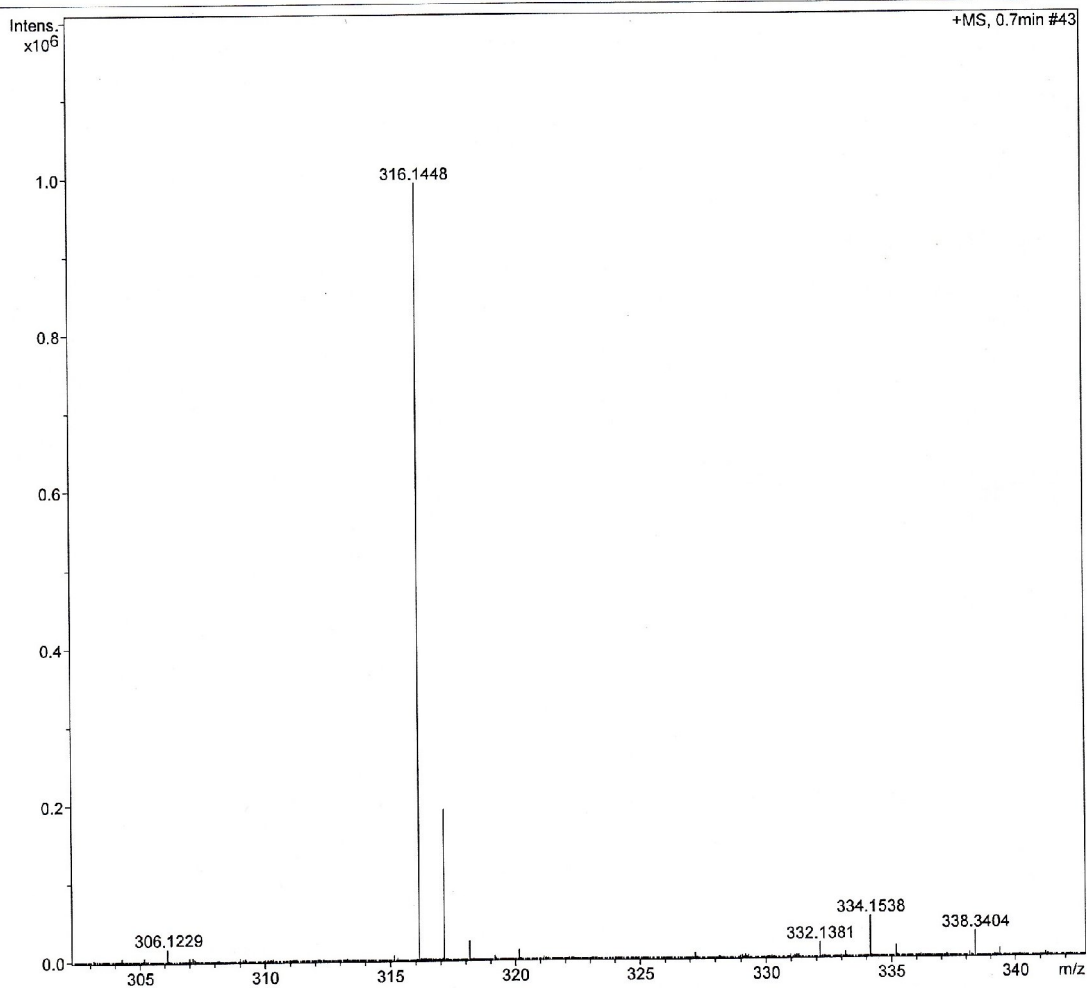
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Comment

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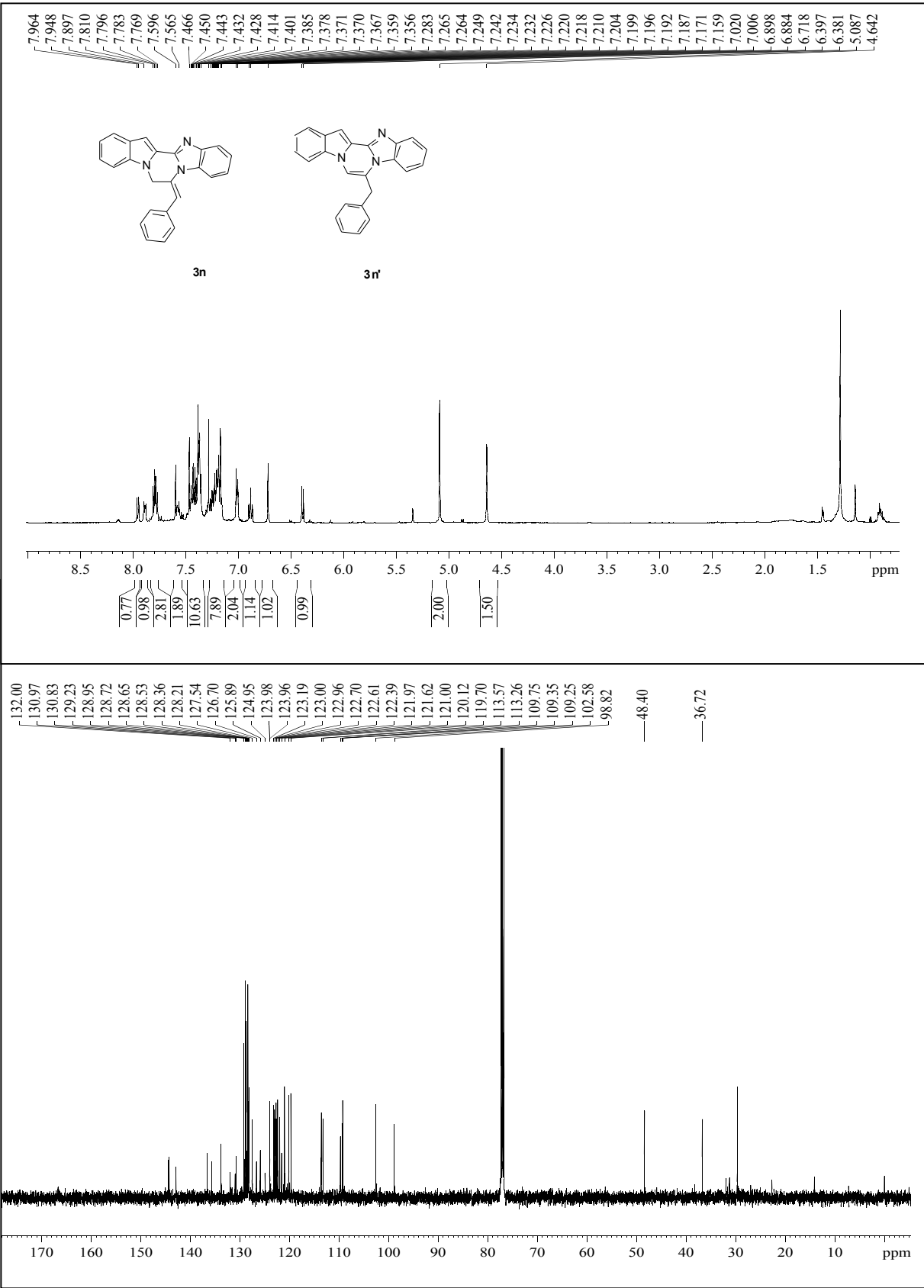
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C spectra of compounds 3n and 3n'



HRMS of 3n and 3n'

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Analysis Info

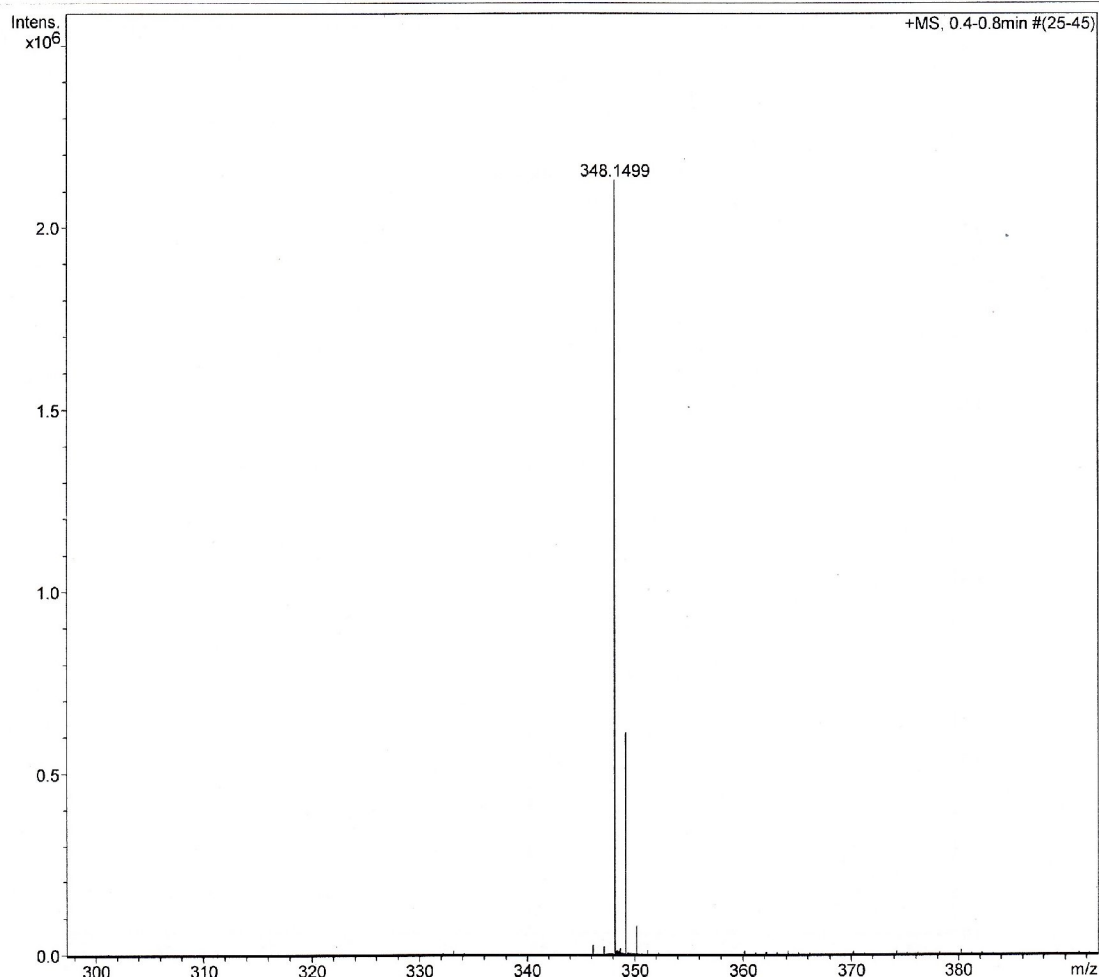
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Acquisition Date 3/28/2013 11:44:23 AM

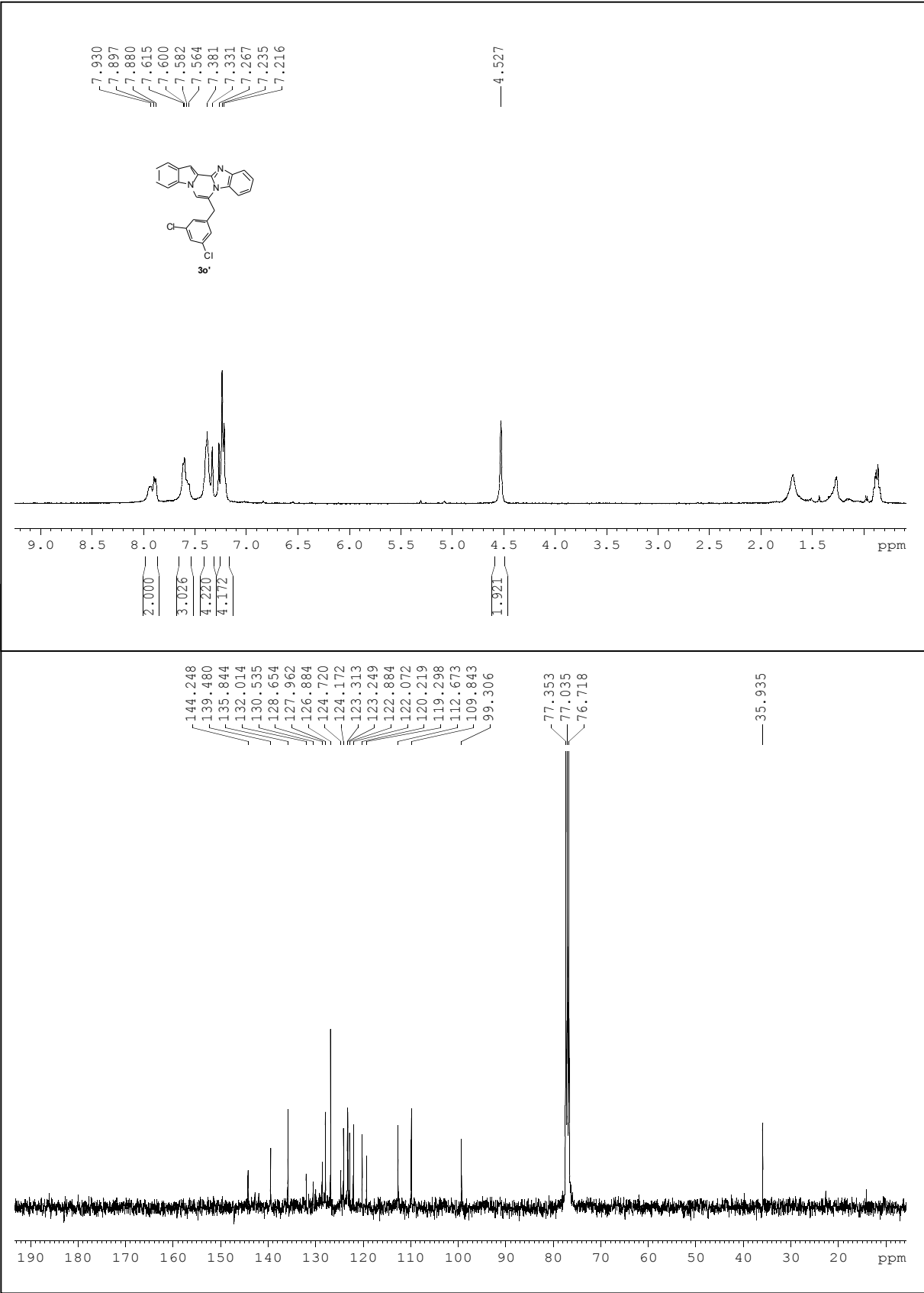
Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

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Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
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Scan End	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C spectra of compound 3o'



HRMS of 3o'

BRUKER MAXIS HRMS REPORT

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Analysis Info

Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SRM-691.d
Method tune_low_Pos.m
Sample Name SRM-691-DCM-MEOH
Comment

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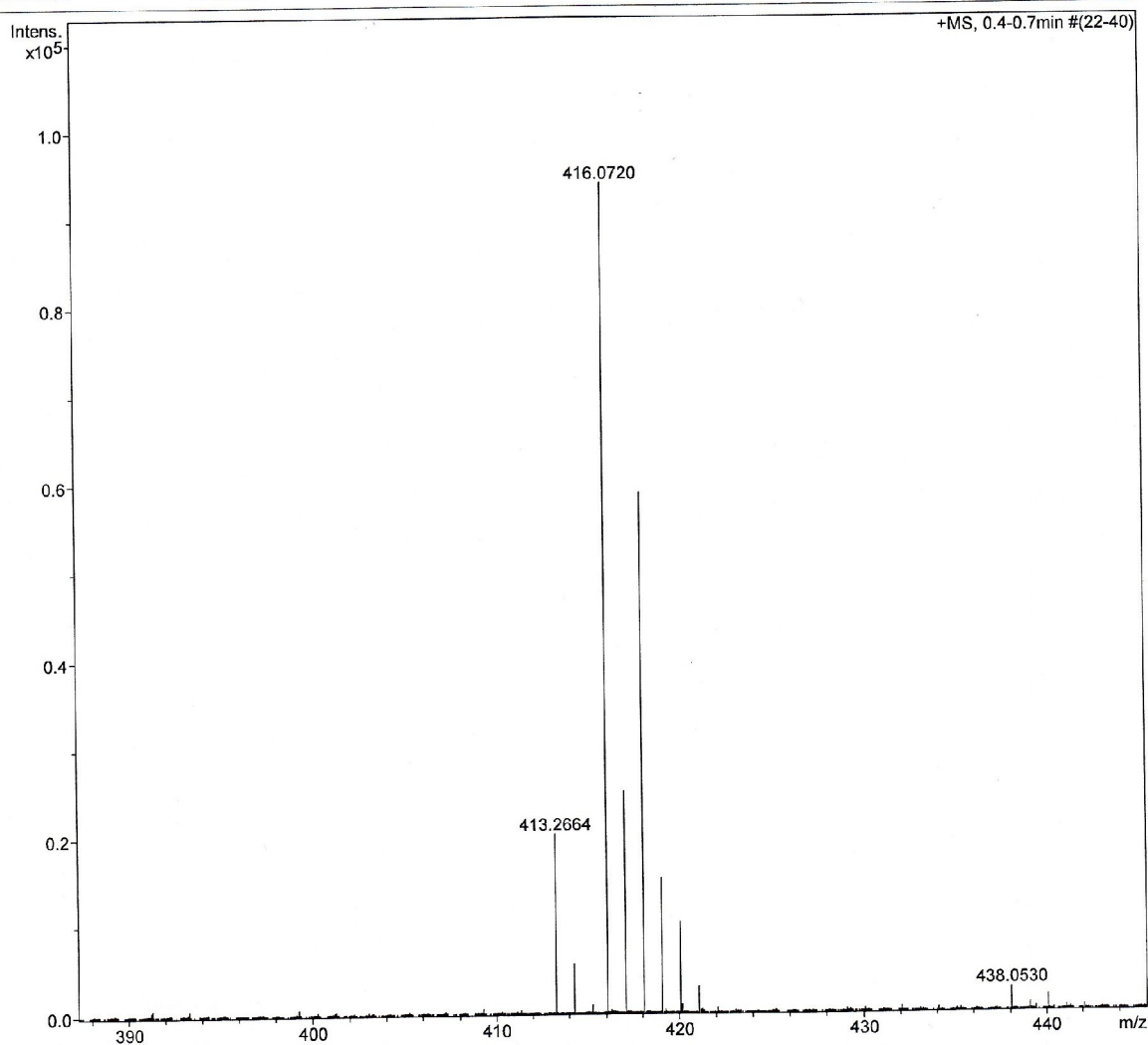
Operator Ramu Sridhar
Instrument maXis 10138

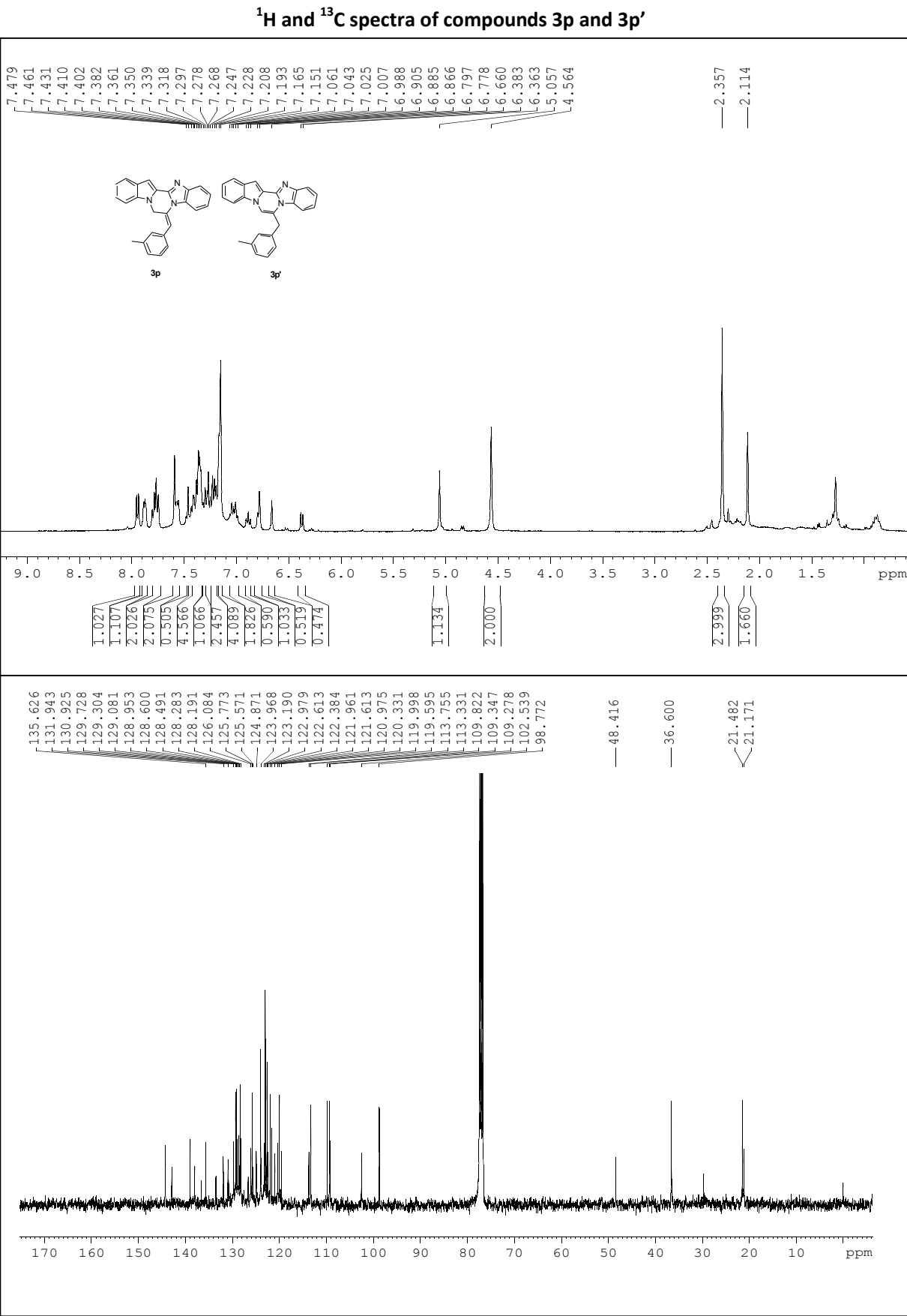
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Scan End 1500 m/z

Ion Polarity Positive
Set Capillary 3800 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 4.4 psi
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste





HRMS of 3p and 3p'

BRUKER MAXIS HRMS REPORT

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Analysis Info

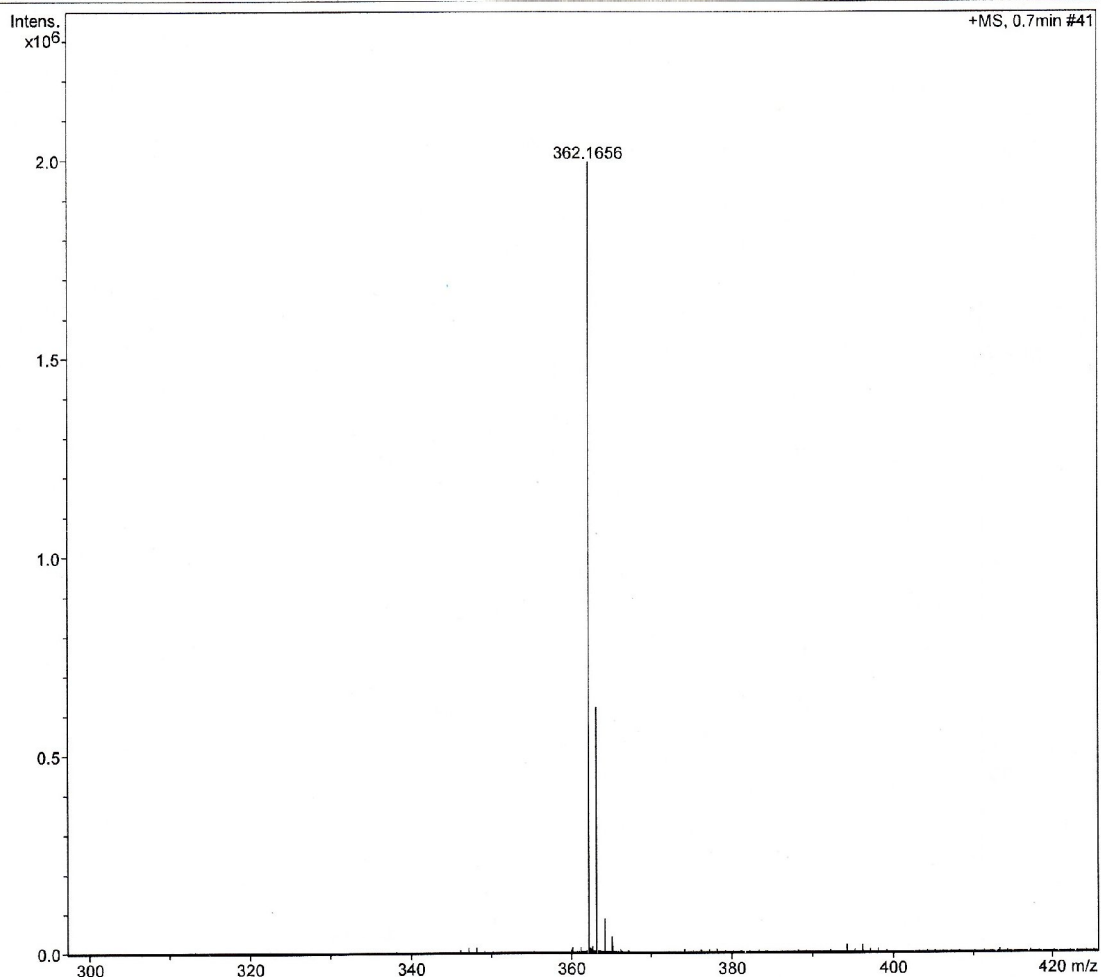
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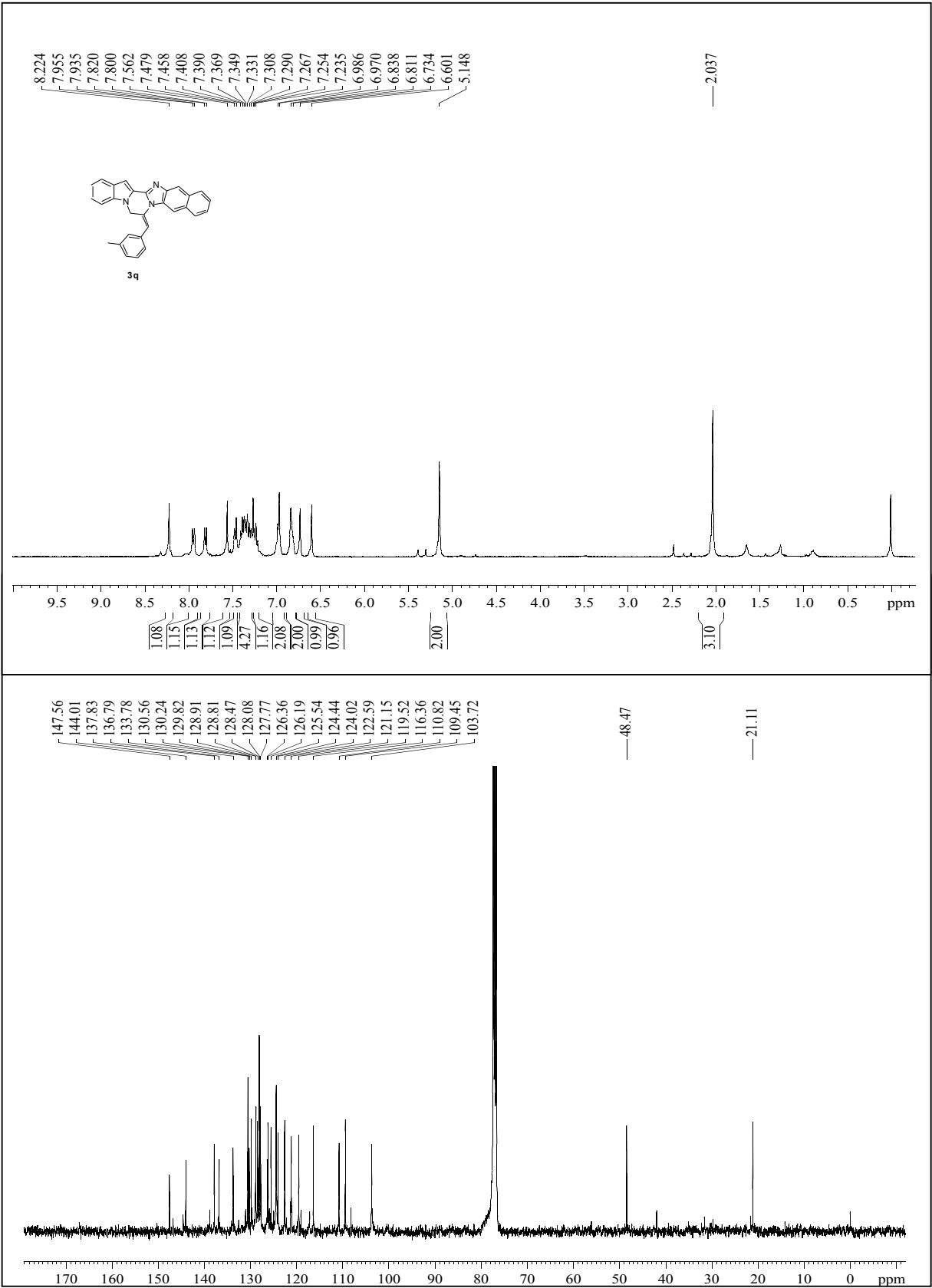
Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

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Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C spectra of compounds 3q



HRMS of 3q

BRUKER MAXIS HRMS REPORT

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University of Hyderabad

Analysis Info

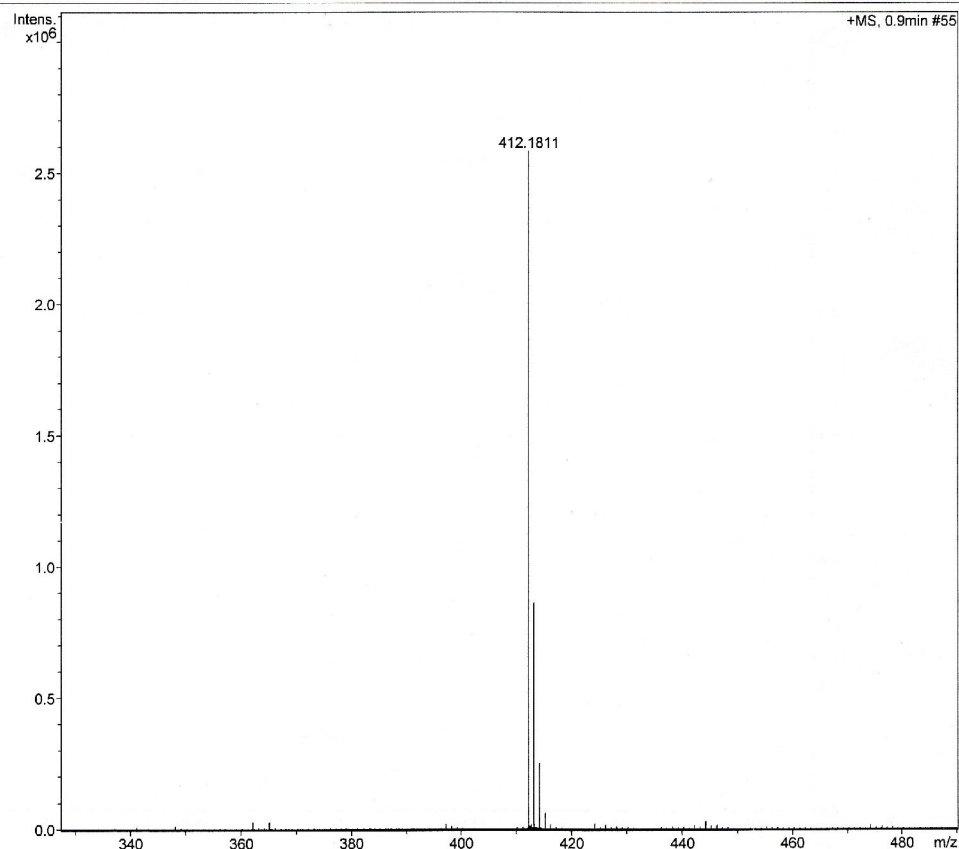
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Sample Name SRM-649dcm-meoH
Comment

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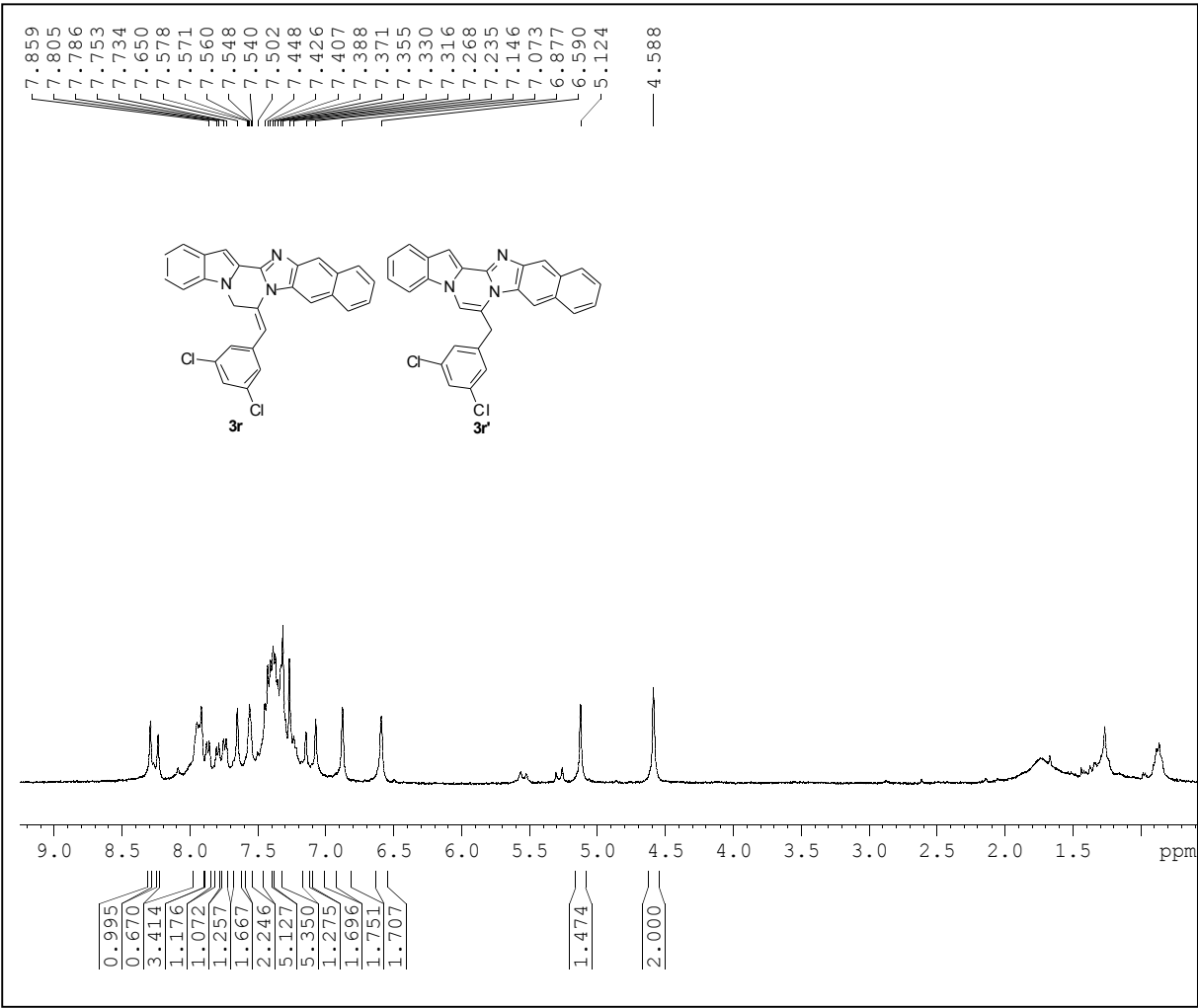
Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
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Scan End	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H spectrum of compounds 3r and 3r'



HRMS of 3r and 3r'

BRUKER MAXIS HRMS REPORT

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University of Hyderabad

Analysis Info

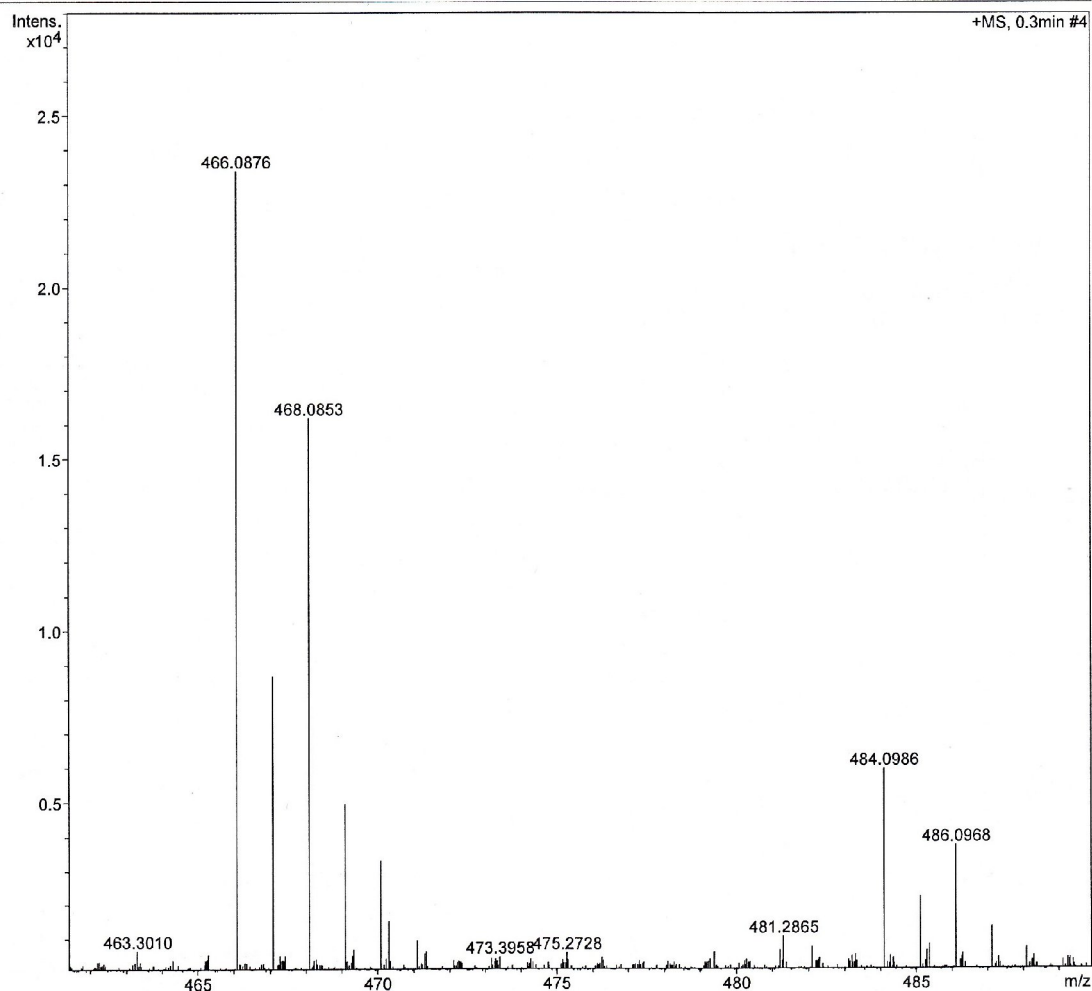
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Method tune_low_Pos.m
Sample Name SRM-695-DCM-MEOH
Comment

Acquisition Date 7/15/2013 3:49:17 PM

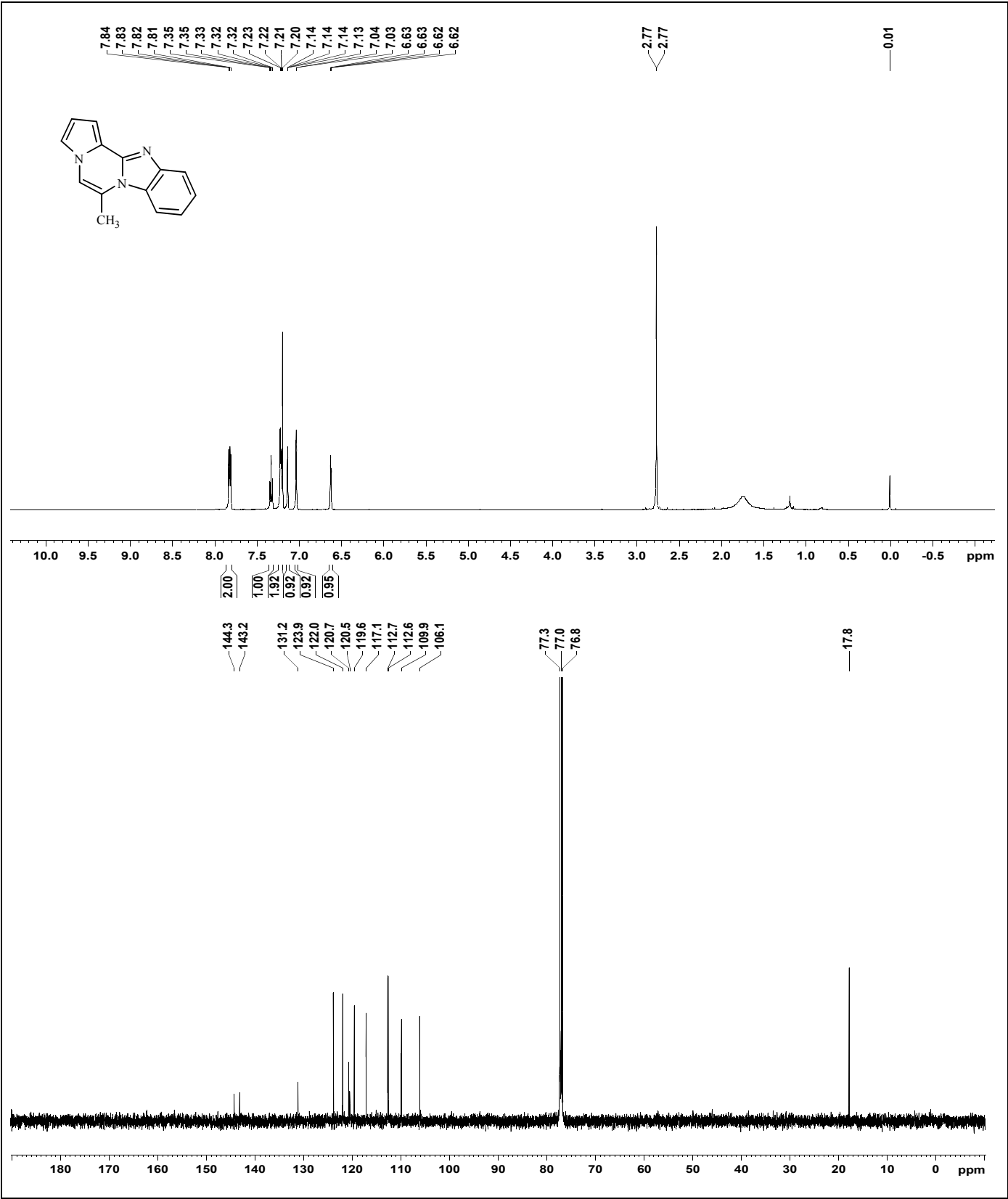
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



1H and 13C Spectra of 5a



HRMS of 5a

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Analysis Info

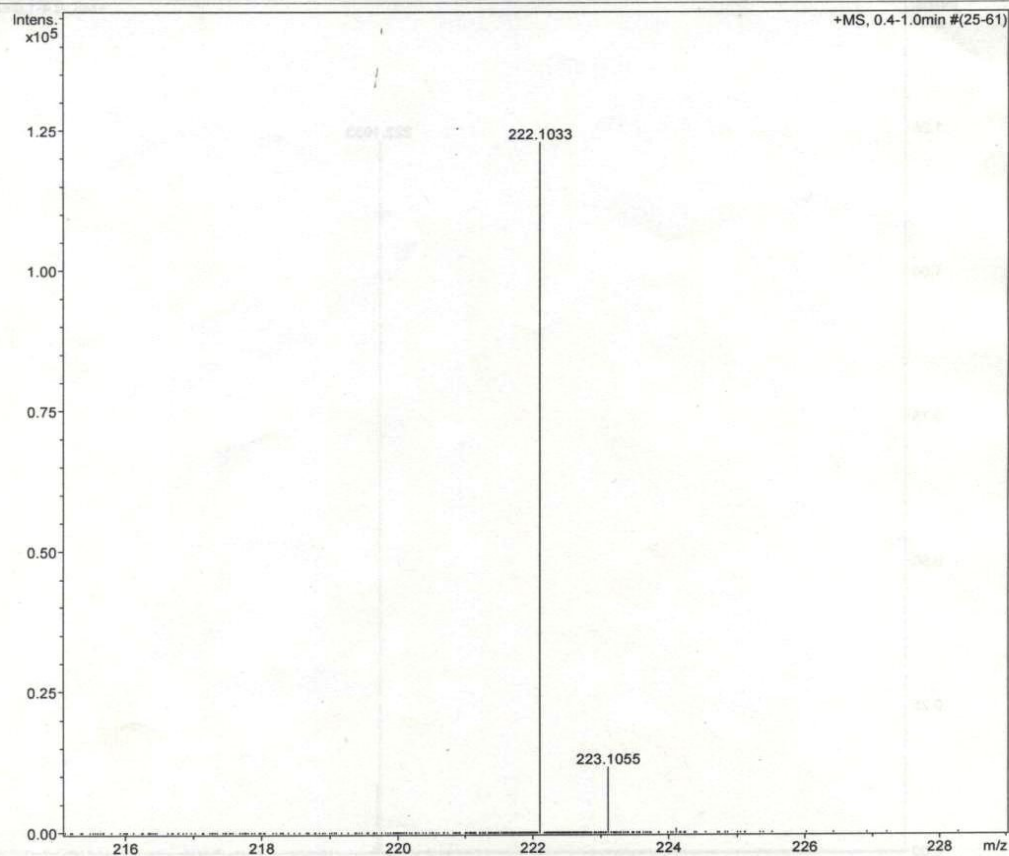
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Comment

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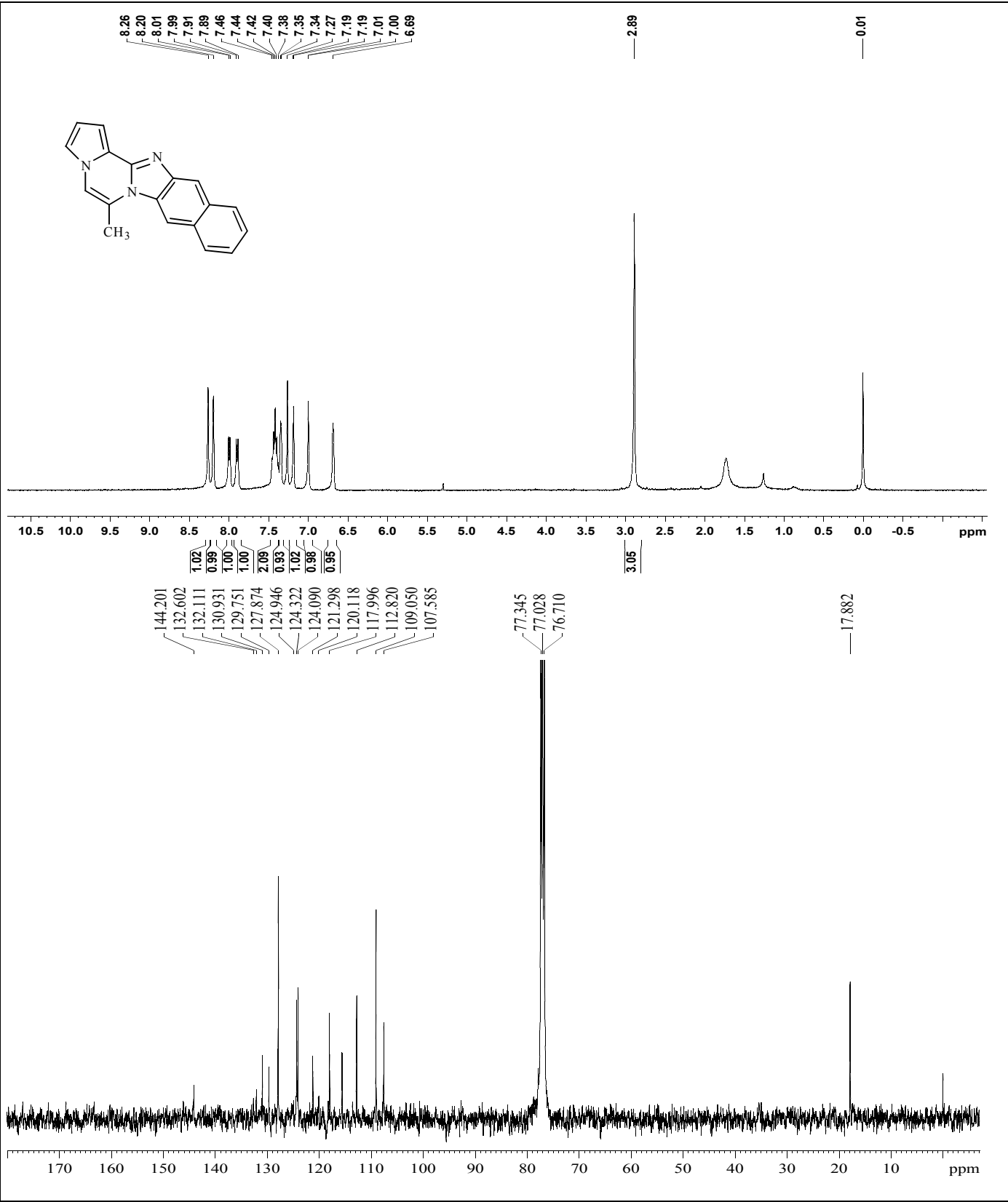
Operator UOH
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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¹H and ¹³C Spectra of 5b



HRMS of 5b

Display Report

Analysis Info

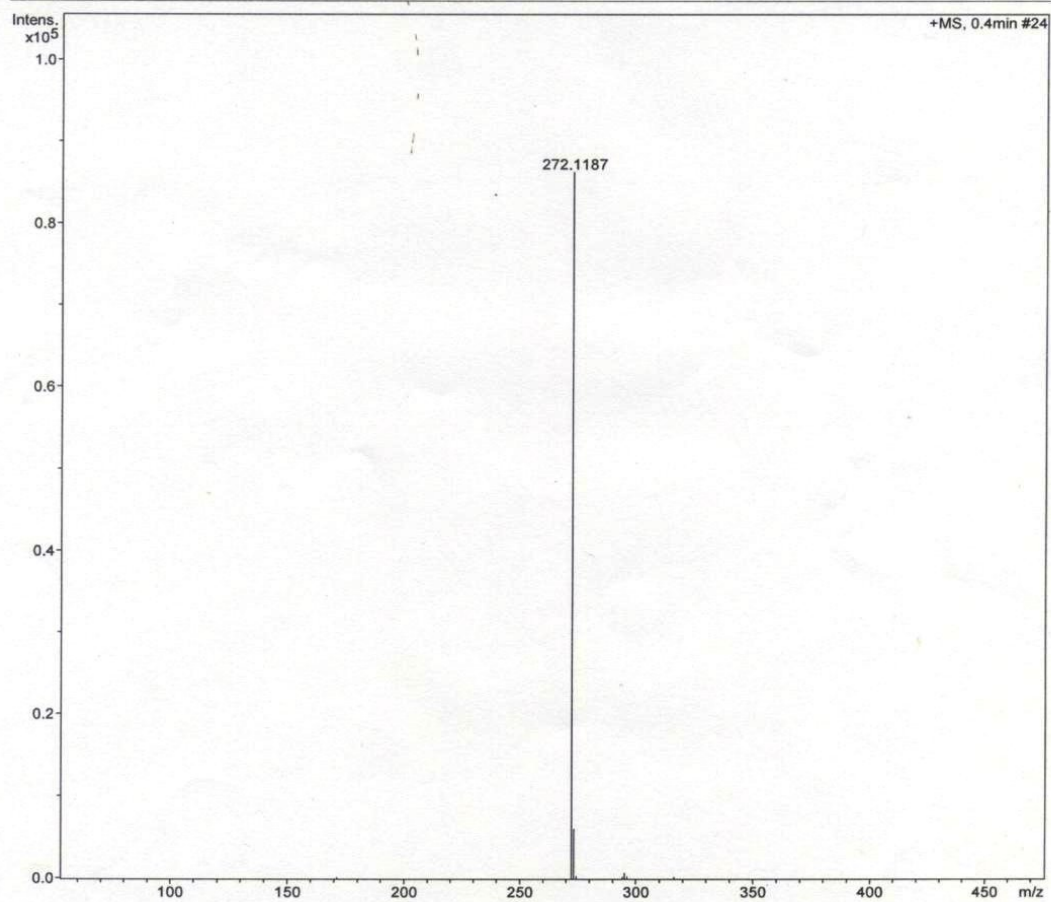
Analysis Name D:\Data\2013\Dr.NAGARAJAN\SRM-SKG-67R.d
Method tune_low.m
Sample Name SRM-SKG-67-DCM-MEOH
Comment

Acquisition Date 1/7/2013 4:40:01 PM

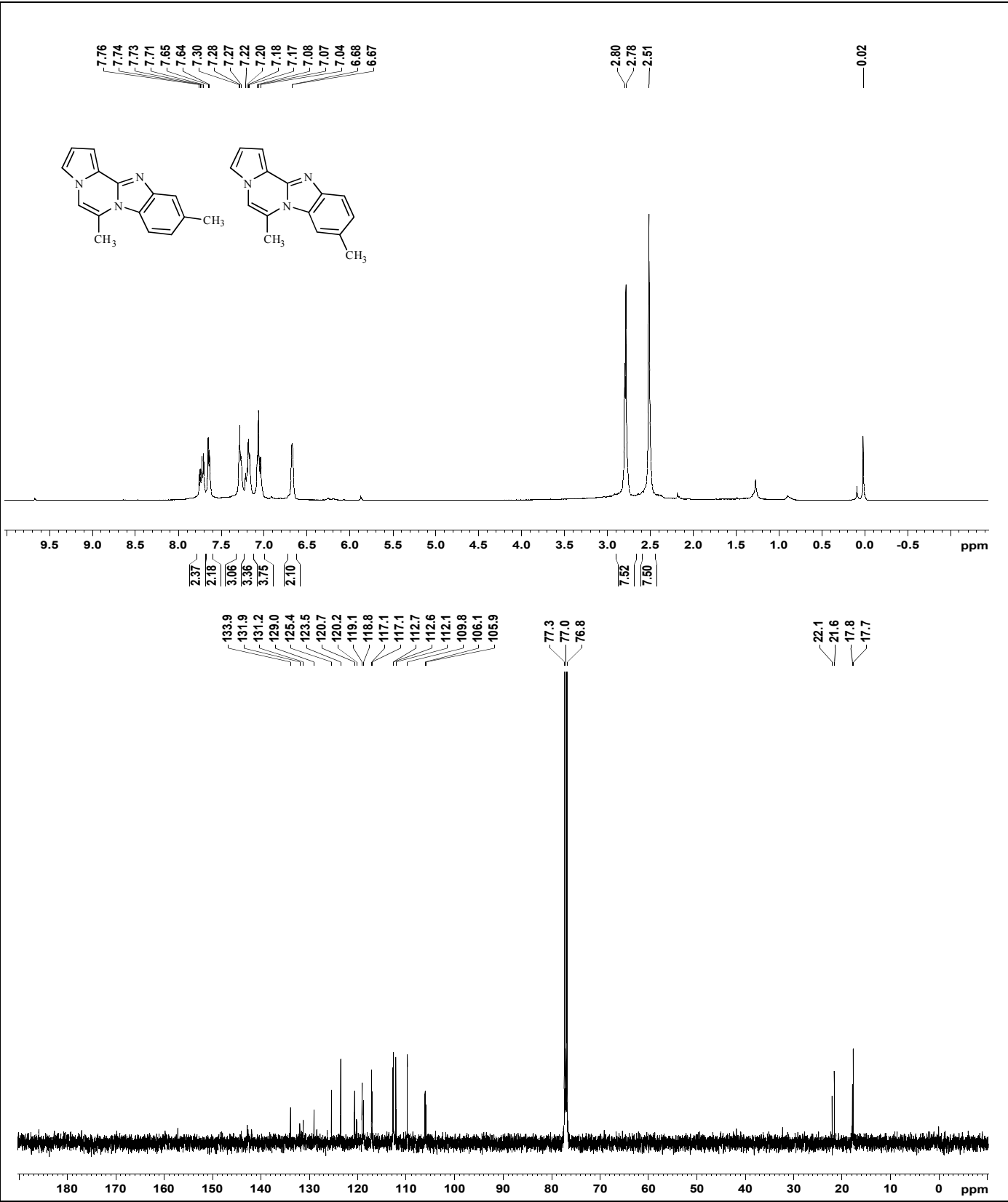
Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 5c and 5c'



HRMS of 5c and 5cc

Display Report

Analysis Info

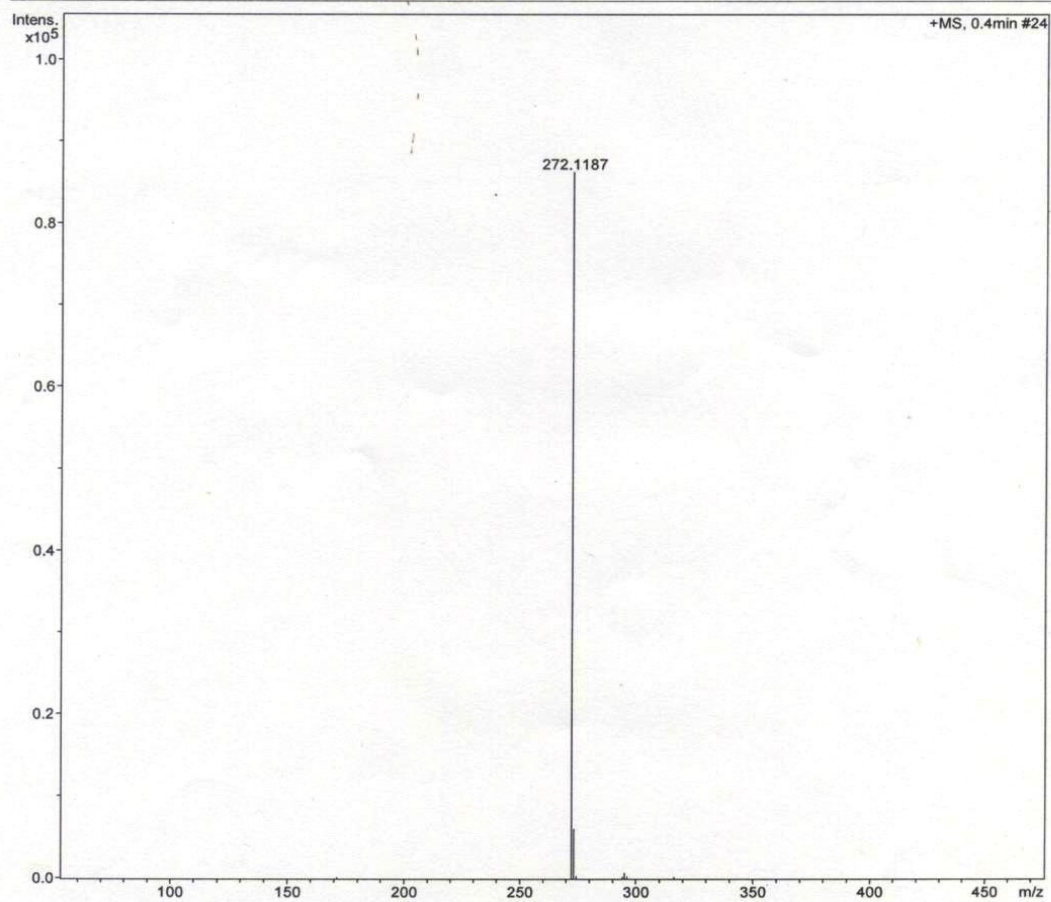
Analysis Name D:\Data\2013\Dr.NAGARAJAN\SRM-SKG-67R.d
Method tune_low.m
Sample Name SRM-SKG-67-DCM-MEOH
Comment

Acquisition Date 1/7/2013 4:40:01 PM

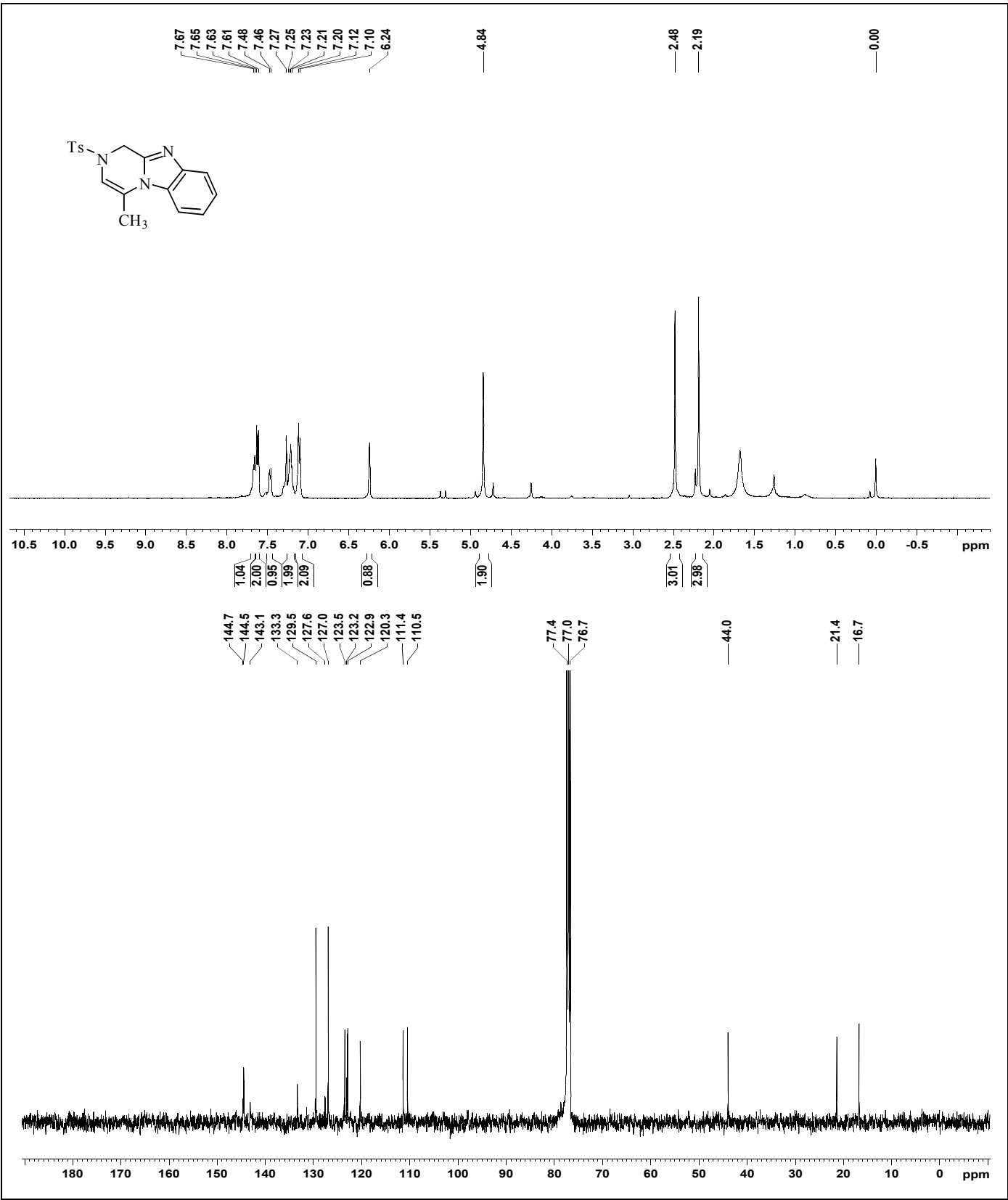
Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 7a



HRMS of 7a

Display Report

Analysis Info

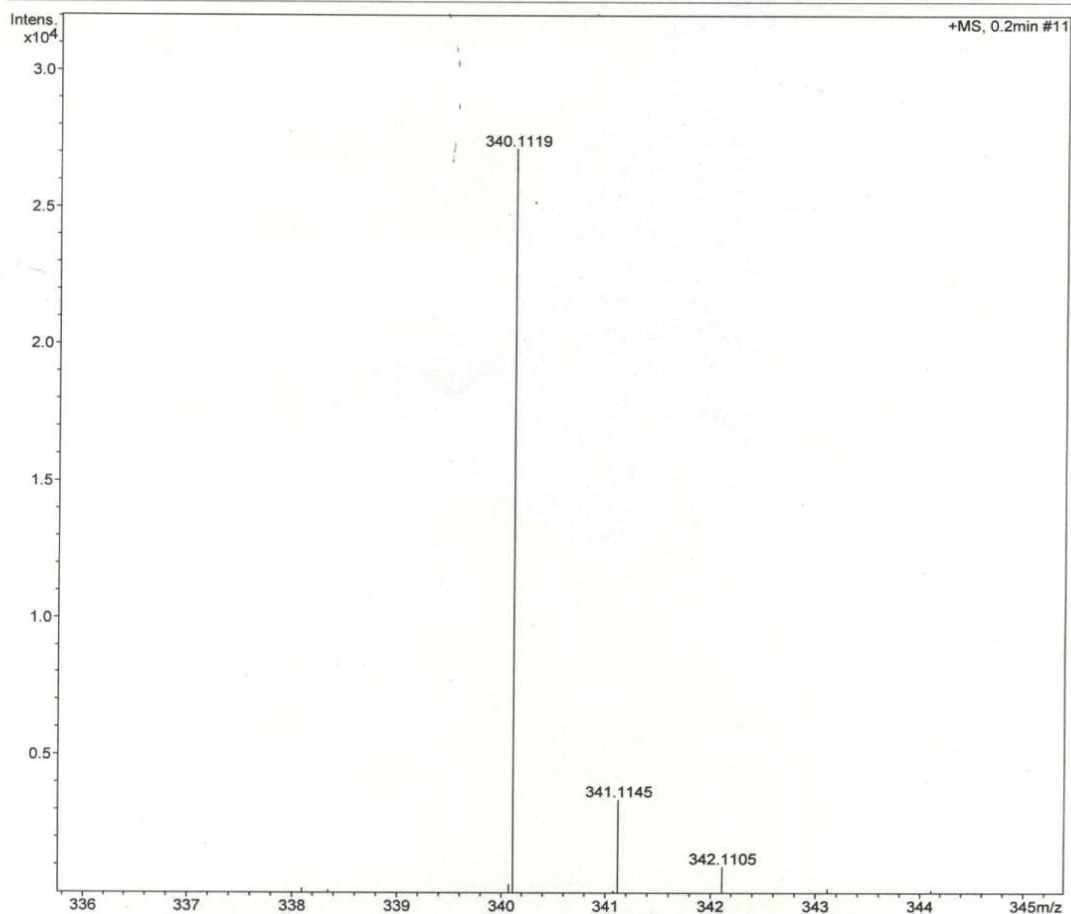
Analysis Name D:\Data\2012\Dr.R.Nagarajan\NOV\SKG-130.d
Method tune_low_Pos.m
Sample Name SKG-130-DCM-MEOH
Comment

Acquisition Date 11/6/2012 4:25:51 PM

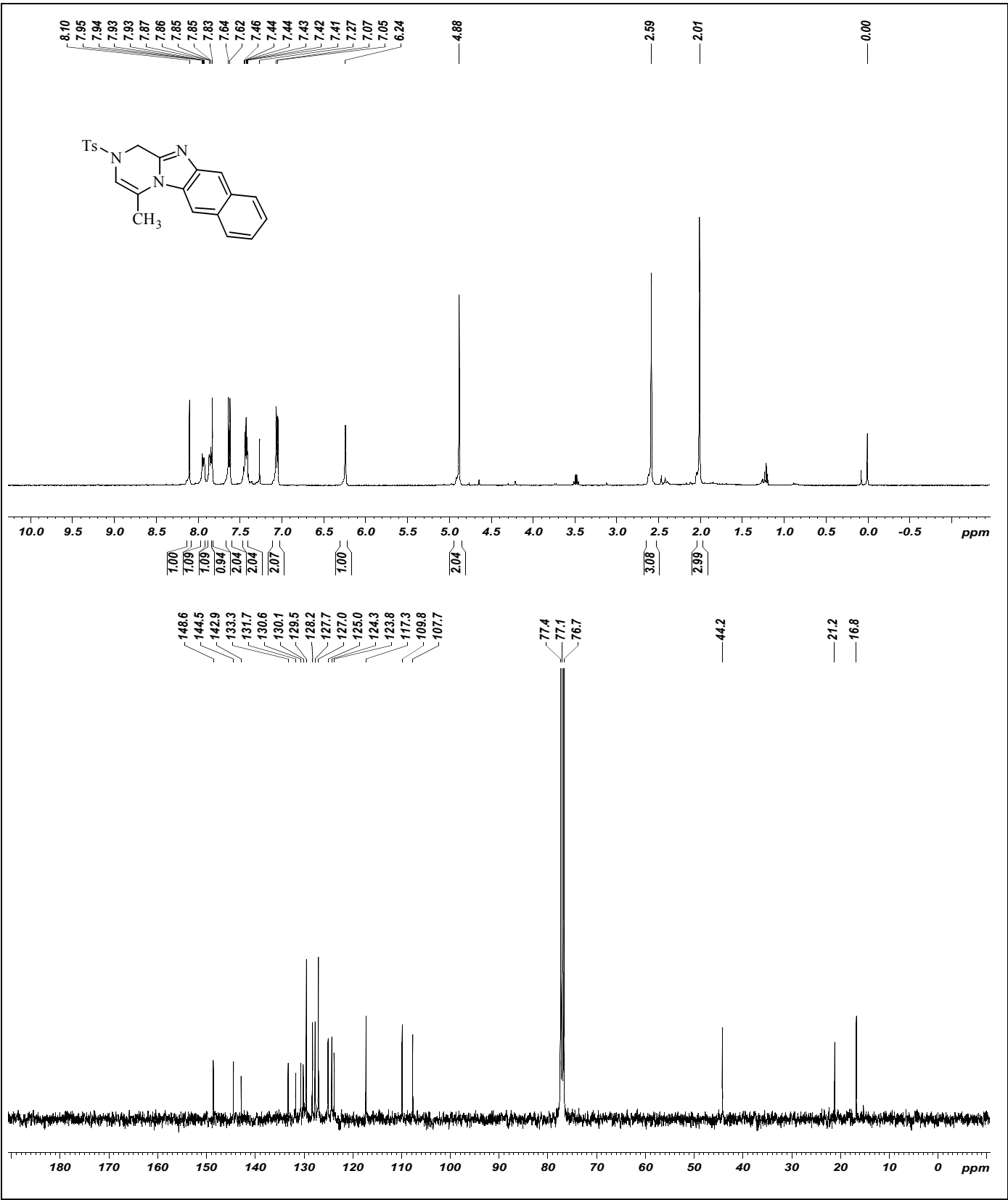
Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 7b



HRMS of 7b

Display Report

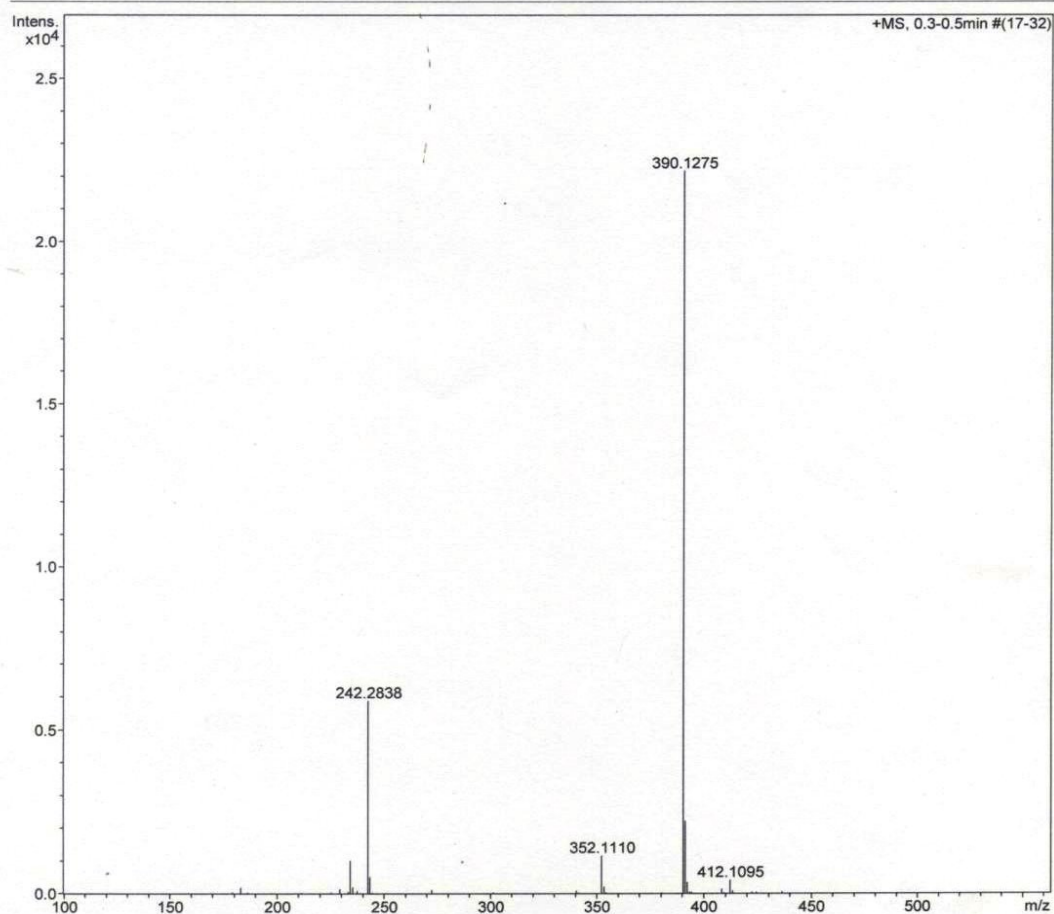
Analysis Info

Analysis Name D:\Data\2013\Dr.NAGARAJAN\JAN\SRM-SKG-149.d
Method tune_low.m
Sample Name SRM-SKG-149-DCM-MEOH
Comment

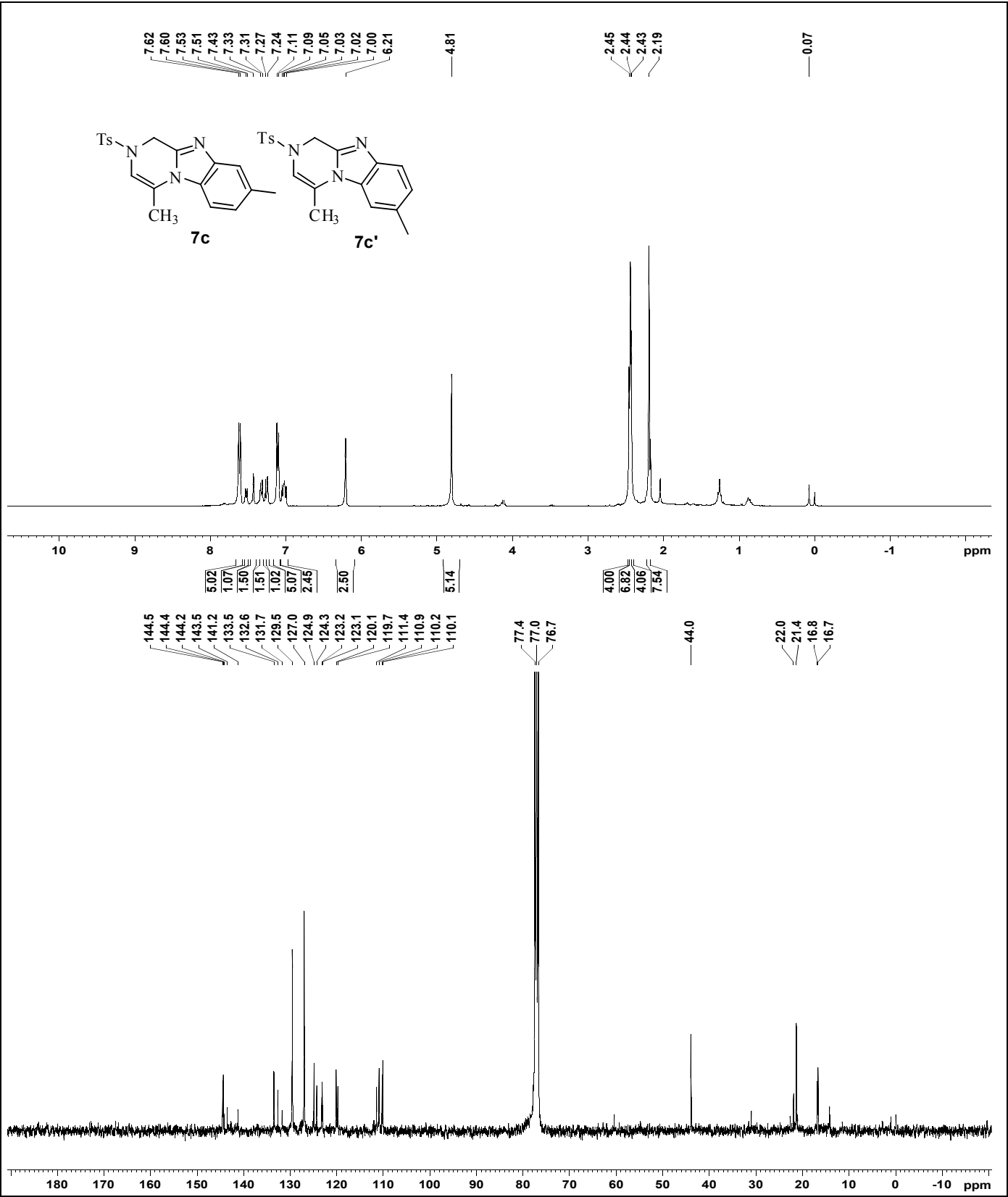
Acquisition Date 1/7/2013 4:58:41 PM
Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C Spectra of 7c and 7c'



HRMS of 7c and 7c'

Display Report

Analysis Info

Analysis Name D:\Data\2013\Dr.NAGARAJAN\SRM-SKG-140.d
Method tune_low.m
Sample Name SRM-SKG-140-DCM-MEOH
Comment

Acquisition Date 1/7/2013 4:49:46 PM

Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste

